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RELATIONS BETWEEN DEPTH OF BURIAL, VITRINITE REFLECTANCE AND GEOTHERMAL GRADIENT

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In wells where the drilled sequence is now at its maximum temperature, relations between depth and vitrinite reflectance show three segments: an upper segment with a linear gradient from 0.2-0.25% Ro at the surface to 0.6-0.7% Ro; a middle segment in which reflectance increases rapidly to c.1.0% R; and a lower segment in which the gradient is again linear but reflectance increases more rapidly than in the upper segment. With a linear scale for depth, the inflection represented by the short middle segment tends to be obscured by the adoption by some authors of a log scale for reflectance.

The depth to the inflection systematically increases with decrease in geothermal gradient, allowing the development of a general diagram relating depth, reflectance and geothermal gradient. In wells where erosion is probable either at the present-day surface or at an unconformity, the general diagram can be used to estimate former maximum depths of burial and paleogeothermal gradients. These estimates, together with the presence of the inflection in the depth/reflectance relation, should be part of the input into modelling of the thermal history of sedimentary basins when reflectance is used in the model. The inflection is the result of the changing chemistry of vitrinite during oil generation, and the contrast between the depth/reflectance gradients above and below the inflection comparably reflects the contrast in vitrinite chemistry.

INTRODUCTION

The increase in vitrinite reflectance (%Ro) with depth, exemplified in wells drilled for hydrocarbons, is not linear over the peat-anthracite rank range. In any one well, the rate of increase is normally greater in that part of the sequence with low-volatile bituminous and higher rank coals (>1% Ro) than in the part with lower rank coals. Because of the non-linearity, some workers, but by no means the majority, have illustrated the depth/reflectance relation by using a log scale for reflectance against a linear scale for depth.

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This usage may introduce a bias into the interpretation, in particular by tending to minimise any marked bend that leads to a greater rate of increase of reflectance with depth and by obscuring the comparison with plots that use a linear scale for reflectance.

Vitrinite reflectance is by no means a precise parameter. Mukhopadhyay (1994) reviewed its use as a maturity parameter, citing many causes of variability and emphasising the need for standardisation of procedures. One of the most important uncertainties lies in the variability of vitrinite composition which introduces difficulties in comparison of wells, particularly those in widely separated regions. Lower reflectance in some vitrinites than in others — "suppression" of reflectance — is now widely recognised (cf. Newman and Newman, 1982; Price and Barker, 1985), and an encouraging technique using fluorescence alteration to compensate for vitrinite variation (Wilkins *et al.*, 1992) is not yet in general use.

In practice, when results from many sources are brought together, a substantial problem lies in differences in reflectance determinations between different laboratories; those cited by Lin (1994), for example, are minimal compared with some recorded in open-file petroleum reports (cf. Sykes *et al.*, 1992, fig. 3). Whereas Lin's comparison used standard samples for all laboratories, separate samples are used where different laboratories have reported on the same well for different oil companies. Problems of inter-laboratory differences and intrinsic variation in vitrinite composition are particularly important when reflectance is determined on a few grains of dispersed organic matter rather than on coal. A further problem lies in the common failure to indicate whether mean maximum or mean random reflectance has been determined, although the difference is slight below 1.0% Ro (cf. Lin, 1994, fig. 5). Finally, in some wells, cavings from higher in the well may contaminate some samples.

In the depth/reflectance plots for all the many wells discussed below, it has been necessary in most cases to read off the reflectance and depth values as accurately as possible from the published diagrams. The consequent lack of precision is considered to introduce only insignificant uncertainties.

The various difficulties, however, should not preclude an attempt to better understand the patterns of depth/reflectance relations, of which Koch (1974) recognised three different types and Robert (1988) recognised four types. Both these authors attributed the differences to differences in thermal history, but neither presented temperature data for the wells that they discussed. Koch did not present reflectance values and Robert showed generalised values, commonly at 0.05% intervals, without the observations on which they were based. Accordingly, it is difficult to judge the validity of their inferences. Additionally, lowered reflectance may result from overpressuring as inferred by Fang *et al.* (1995). Sykes *et al.* (1991), noting low vitrinite reflectance in coals below an overpressured zone in the *Tane-1* well (Taranaki Basin, New Zealand), attributed it to the retention of high moisture in the coals, citing a general study of reflectance and moisture in isorank New Zealand coals by Suggate and Lowery (1982).

In order to relate reflectance to geothermal gradient, it is necessary to use wells that provide temperatures and reflectance values that derive, so far as can be judged, from the depths of burial and thermal regimes under which the ranks (and hence the reflectance) were set. The simplest case is where the stratigraphy indicates that subsidence is continuing, particularly if this is supported by near-surface reflectance values of 0.25±0.06% in keeping with reflectance values for peats and for lignites buried <250 m (Suggate, 1990, fig. 7), and with the extrapolated surface values in the wells shown in Fig. 1. Particularly useful are those wells for which temperature data are available, despite the difficulties of correcting bottom-hole temperatures. Present-day temperature gradients may also be applicable where subsidence ended in very late geological time and the amount of erosion can reasonably be estimated. In the following discussion, such cases are used in producing a generalisation relating vitrinite reflectance to maximum depth of burial and geothermal

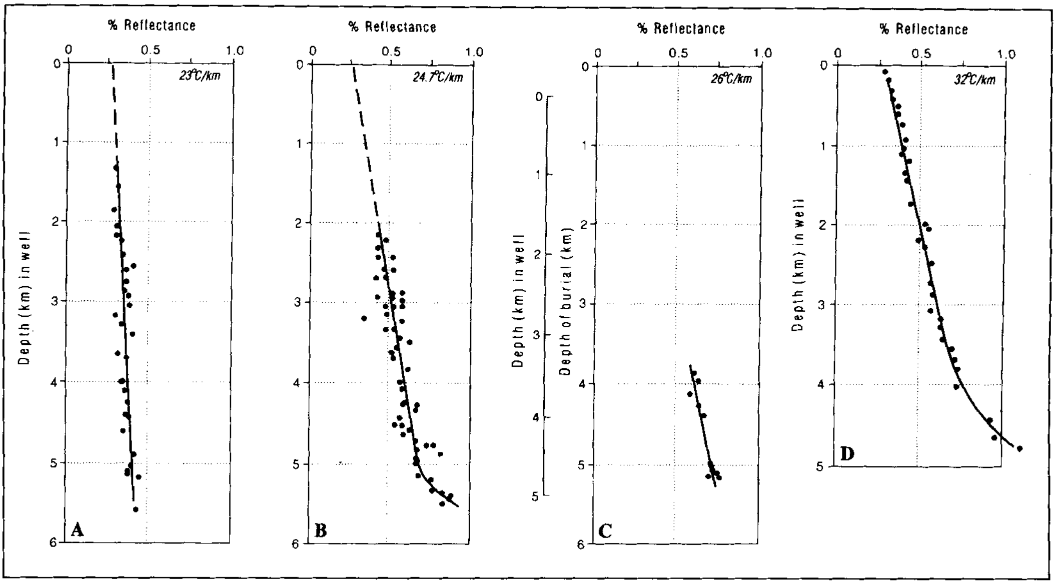

Fig. 1. Depth/reflectance relations.
A: *Site V*, Ventura Basin (data from Bostick *et al.*, 1978). B: *Point au Fer*, Louisiana (data from Heling and Teichmüller, 1974). C: *Kapuni Deep-1*, Taranaki Basin, New Zealand. D: *COST-1*, offshore Texas Gulf Coast (data from Waples, 1981).

gradient, and that generalisation is used to make estimates of past thermal regimes and amounts of erosion. The geothermal gradient is stated for some wells, and "corrected" bottom-hole temperatures for others. Uncertainties arise in comparing wells with temperature data that have been corrected in different ways, but these are regarded as minor in the context of the wide range of geothermal gradients considered here.

Relations between vitrinite reflectance, depth of burial and geothermal gradient established for present-day thermal regimes will also have applied in ancient sedimentary basins prior to uplift and erosion. Reflectance values will in effect have been fossilised unless greater temperatures were later attained through either re-burial or increased heat flows. In these cases, the effects of the more recent thermal regimes will have obliterated the effects of the initial regime.

Vitrinite reflectance (within its considerable limitations) is here accepted as a maximum thermometer. Under geological conditions, durations at maximum temperatures are sufficiently long for the time factor to be accepted as of negligible account. A significant effect of time is yet to be demonstrated by, for example, a comparison of reflectance profiles in basins with similar present-day maximum depths of burial and temperatures but with substantially contrasting rates of sedimentation.

WELLS USED FOR GENERALISING Ro/DEPTH RELATIONS (Table 1)

Ventura Basin, California, USA (Fig. 1A)

Two wells <5 km apart, together designated *Site V* by Bostick *et al.* (1978), bottomed in Pliocene rocks at depths of 5,394 and 7,710 m. Present-day burial depths were judged to be "maximal" on the basis of structure and stratigraphy, and the geothermal gradient was given as 23°C/km. The mean random reflectance value at a depth of 1.3 km was 0.3%; at a depth of 5 km it was only 0.4%. No distinction was made between types of

Table 1. Wells used for generalising relations between depth, reflectance and geothermal gradient.

Well	Age range	——Minimum Ro—— Ro* %	Depth (km)	Age	Geotherm. Gradient (°C/km)	Surface Temp. (°C)
USA						
Cost-1, Gulf Coast	Mio.-Pleist.	0.3	0.1	Pleist.	32	18
Site V, Ventura B.	Plio.-Quat.	0.3	0.13	Quat.	23	23
Point au Fer, Lo.	Mio.-Quat.	0.42	2.15	Late Mio.	24.7	23**
Rhine graben						
Dudenhofen-2		0.6	1.4	77	10	
Hähnlein West-2	Oligo.-Plio.	0.2	0.2	Plio.	48	10
Harthausen-1	Meso.-Mio.	0.25	0.35	Mio.	67	10
Hessbach-2		0.55	0.75	77	10	
Karlsdorf-1		0.65	1.4	67	10	
Landau-2	Eo.-Mio.	0.2	0.35	Mio.	77	10
Landau-3		0.2	0.25	71	10	
Landau-9		0.55	1.2	77	10	
Sandhausen-1	Oligo.-Mio.	0.25	0.65	Mio.	42	10
Scheibenhardt-2	Meso.-Mio.	0.3	0.3	Mio.	77	10
New Zealand						
Kapuni Deep-1	Paleoc.-Pleist.	0.6	3.9	Eo.	26	12

* *Based on inferred Ro/depth relation, not on individual sample.*
** *Estimated.*

vitrinite, however, with the result that the reliability of individual determinations was less than the apparent total downhole increase in reflectance. Further, Price and Barker (1985) maintained that suppression of vitrinite reflectance was prevalent in Los Angeles Basin sequences similar to those discussed by Bostick *et al.* (1978).

Terrebonne Parish, *Point au Fer* well, Louisiana, USA (Fig. 1B)

Heling and Teichmüller (1974, fig. 4) presented a depth/reflectance plot for this well (reproduced by Robert, 1988, fig. 36), also showing a corrected final temperature at 5,334 m in late mid-Miocene rocks near the bottom. The average temperature gradient is 24.7°C/km, assuming 23°C at the surface. An approximate temperature at 3,048 m gives 24.6°C/km. If the linear reflectance gradient between 2,000 and 4,000 m is extrapolated to the surface, a near-surface sample would have a reflectance of 0.25% Ro. The depth/reflectance relation (Fig. 1B) is only slightly different from that shown by Heling and Teichmüller (1974),but shows a more pronounced inflection near the bottom of the well.

Kapuni Deep-1, Taranaki Basin, New Zealand (Fig. 1C)

This well was drilled at the same site as *Kapuni-1*. Mean maximum reflectance values from Lowery (1988) are reproduced in Fig. 1C. Minor erosion of Late Pliocene and Quaternary sediments, with a subsequent covering of volcanics, has left a net loss of c.0.5 km from the top of the sequence (Elphick and Suggate, 1964), but the geothermal gradient is assumed not to have changed significantly from the present 26°C/km. Although the depth/reflectance relation depends on rather few observations and applies to depths of burial of only 3.8 to 5.2 km in Eocene and Paleocene rocks, it is significant in showing a gradient which is very similar to that found in younger rocks in the *Point au Fer* well (Fig. 1B); but there are too few data points to be able to show an inflection in the relation such as that shown at *Point au Fer*.

COST-1, offshore Gulf Coast, USA (Fig. 1D)

Waples (1981, figs 7.8) figured data points for this well, using a semi-log plot. Burnham and Sweeney (1989, fig. 10) cited Waples (1981) as the source of their data, but the data points are not precisely the same; the Waples data are accepted here. The sequence is continuous from mid-Miocene to late Quaternary, and the reflectance values

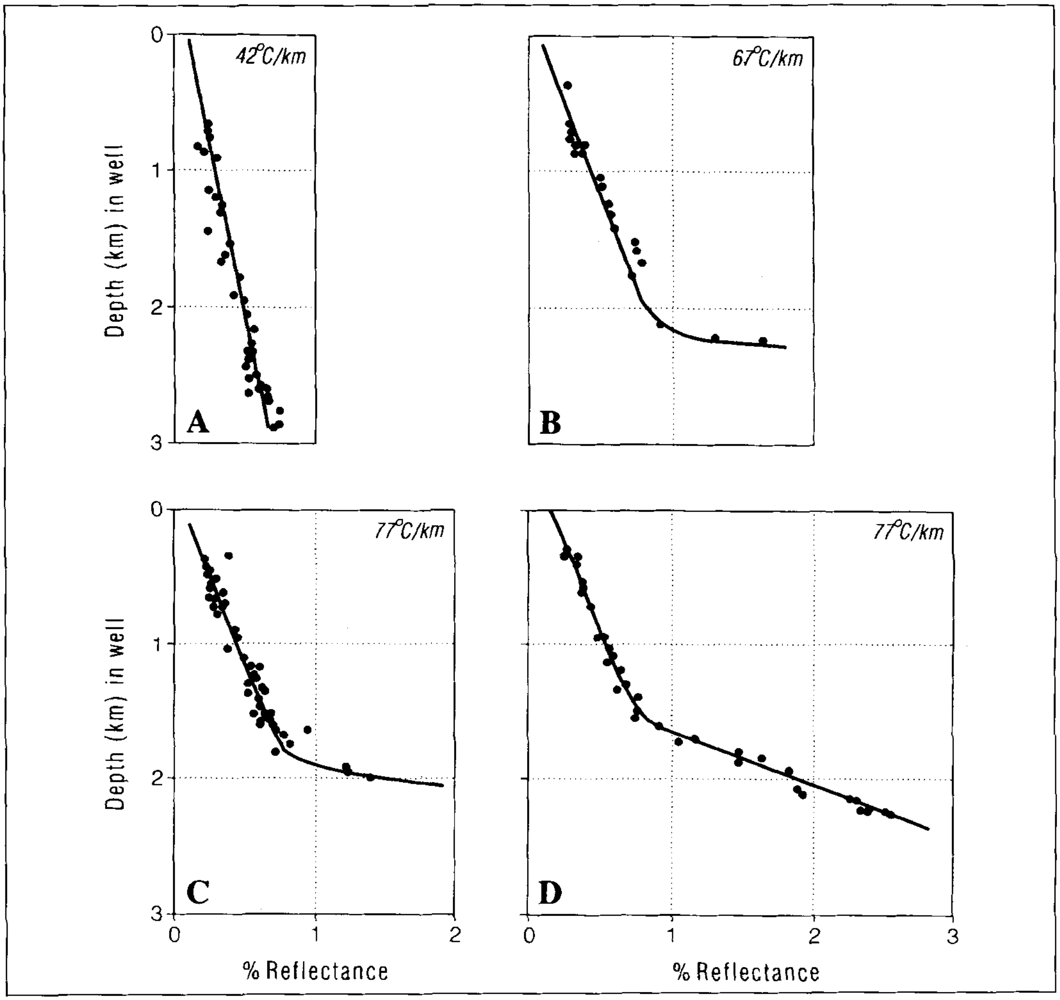

Fig. 2. Depth/reflectance relations in four Upper Rhine Graben wells.
A: *Sandhausen-1;* B: *Harthausen-1;* C: *Landau-2;* D: *Scheibenhardt-2.*
Data from Teichmüller (1979).

extrapolate to 0.25% at the surface. Accordingly, it provides a good depth/reflectance relation related to a geothermal gradient "assumed constant at 1.75°F/100 ft [32°C/km], which is the present day gradient at the bottom of the well" and "a surface temperature taken as 65°F [18°C]" (Waples, 1981, p. 104).

Upper Rhine Graben wells, Germany (Fig. 2)

Teichmüller (1979) and Robert (1988) have published data for numerous wells in the Upper Rhine Graben. Geothermal gradients in the area are high or very high in most areas (Teichmüller, 1979, table 1), and Teichmüller and Teichmüller (1979, p. 109) inferred that "*the high heat flow in wells near Landau and Scheibenhardt has been active for not longer than 2-3 million years before the present*". Reflectance values extrapolate to 0.25% or less at the surface, and assuming that the present geothermal gradients in the region are maxima, the wells provide depth/reflectance gradients for the present-day

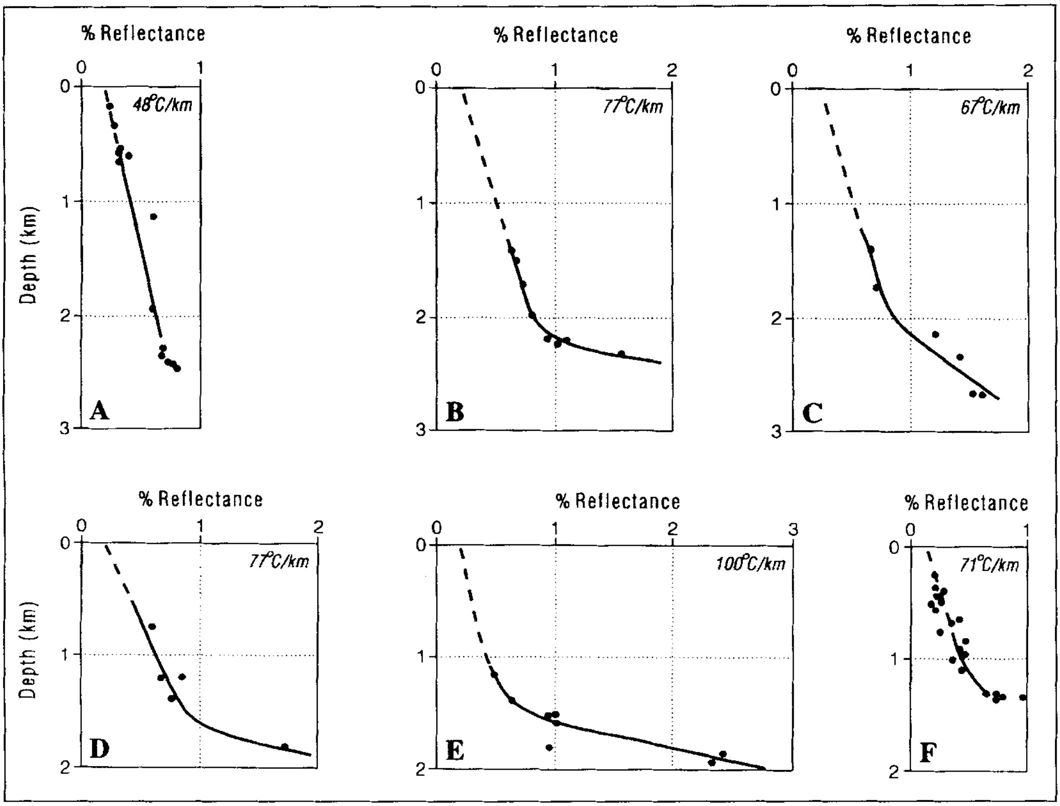

Fig. 3. Depth/reflectance relations in six Upper Rhine Graben wells.
A: *Hähnlein West-2;*B: *Dudenhofen-2;* C: *Karlsdorf-1;* D: *Hessbach-2;* E: *Landau-9;*
F: *Landau-3.* Data from Teichmüller (1979).

geothermal gradients, even though the top sediments are of Miocene or Pliocene age. Teichmüller (1979) figured most prominently four wells (Fig. 2): *Harthausen-1, Landau-2, Sandhausen-1* and *Scheibenhardt-2.* By using figs 3, 5 and 6 of Teichmülller (1979), six additional wells with fewer data points are shown on Fig. 3A-F. Geothermal gradients range from 100°C/km to 42°C/km, with four at 77°C/km and two at 67°C/km, which are averaged in Fig. 4A and B. A set of depth/reflectance profiles for the Upper Rhine Graben wells is shown on Fig.4C. At 100°C/km, 77°C/km and 67°C/km, there are clear inflections in the gradients in the 0.7%-1.0% Ro range. Only at the lower geothermal gradients — 48°C/km and 42°C/km — are there no inflections, but the Ro values only just reach 0.7%. Only *Landau-3*, at 71°C/km, shows an inflection at <0.7% Ro, but as the highest Ro value is <1.0% the inflection is not well controlled.

A generalised depth/reflectance/geothermal gradient diagram

With geothermal gradients of 23°C/km, 24.7°C/km and 26°C/km, the *Site V, Point au Fer* and *Kapuni Deep-1* wells (Fig. 1) might be expected to show closely similar depth/reflectance relations. Both the geothermal and reflectance gradients are lowest at *Site V*, but only its reflectance gradient is markedly lower than for the other two. Because of uncertainties noted above relating to *Site V*, and because the *Point au Fer* and *Kapuni Deep-1* gradients are closely similar, these latter two are preferred, and *Site V* is not used in developing a generalised diagram. *Point au Fer* shows a marked inflection in the 0.7%

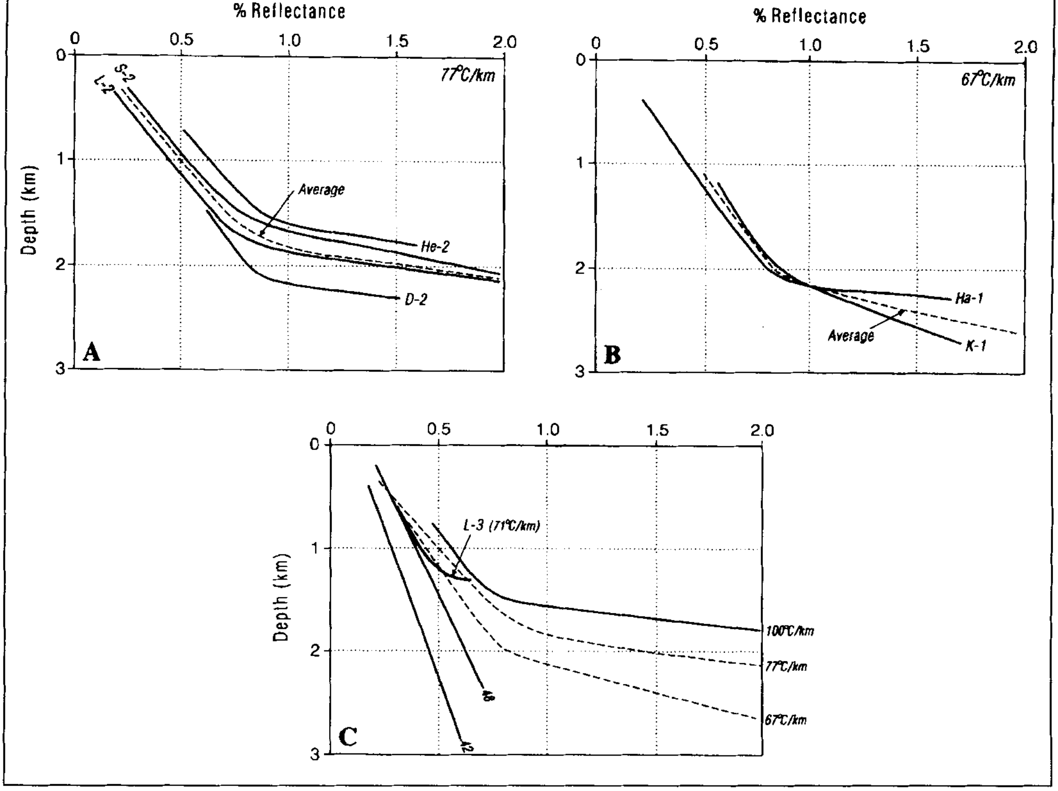

Fig. 4. Generalisations of depth/reflectance relations in Upper Rhine Graben wells.
A: At 77°C/km: *He-2 = Hessbach-2; L-2 = Landau-2; D-2 = Dudenhofen-2.*
B: At 67°C/km: *Ha-1 = Harthausen-1;* K-1 = *Karlsdorf-1.*
C: At gradients from 100°C/km to 42°C/km, from Figs 2, 3 and 4A,B; *L-3 = Landau-3.*

to 1.0% Ro range, but the well was not deep enough to provide a higher rank depth/reflectance relation. *COST-1*, with a geothermal gradient of 32°C/km, shows a rather gentle inflection from 0.7% to 1.0% Ro, but as its reflectance values reach only 1.15%, the high rank gradient is not well controlled. The set of relations for the Upper Rhine Graben wells (Fig. 4C), but excluding *Landau-3*, is used for the higher geothermal gradients.

Regardless of the geothermal gradient, reflectance appears to increase linearly with depth up to c.0.7% Ro, and the rate of increase of reflectance then increases rapidly up to a value of c.1.0%. The subsequent rate of increase is linear with depth but the rate is greater than in the initial phase. The 0.7-1.0% Ro range is that over which atomic H/C ratios decrease after being more or less uniform at lower ranks, consequent upon the release of oil. These effects can be regarded as primarily dependent on temperature increase, and accordingly the temperatures at 0.7% Ro and 1.0% Ro are calculated from the different geothermal gradients and depths, taking into account the surface temperatures (Table 2); for the higher geothermal gradients, temperatures at 2.0% Ro are also calculated. The ranges of calculated temperatures at the successive reflectance values are reasonably small, considering the difficulties associated with reflectance determinations from a wide range of sources, and the small number of critical observations in some wells. The

Table 2. Estimated temperatures at Ro 0.7%, 1% and 2%.

Well	*Surface Temp. (°C)*	*Geotherm. Gradient (°C/km)*	*Ro 0.7%*		*Ro 1%*		*Ro 2%*	
			Depth (km)	*Temp. (°C)*	*Depth (km)*	*Temp. (°C)*	*Depth*	*Temp.*
Landau	10	100	1.40	150	1.57	167	1.80	190
(see Fig. 4)	10	77	1.45	123	1.83	151	2.12	173
(see Fig. 4)	10	67	1.66	121	2.16	155	2.62	186
Hähnlein West-2	10	48	2.30	120				
COST-1, Gulf Coast	18	32	3.70	136	4.65	167		
Kapuni Deep-1	12	26	4.85	138				
Point au Fer	23	24.7	4.90	144	5.60	160		
Average				133		160		183

average temperatures from Table 2 are accepted in constructing a generalised depth/ reflectance/ geothermal gradient diagram (Fig. 5).

Minor difficulties arise from differences of surface temperature, from the variability of reflectance at the initiation of diagenesis, and from the variations of reflectance determinations between laboratories. Further, it is commonly not stated whether the presented reflectance values are mean values (though this will be usual), mean random values or mean maximum values. These problems, however, cannot all be taken into account, and only presented data can be used. It is not practical to determine the variations of reflectance at the surface deriving from differences of surface temperature, and 15°C and 0.25% Ro are adopted for the generalisation (Fig. 5).

If Fig. 5 has general validity, and especially if the effects of time are minimal, the depth/reflectance relations should be generally similar in wells for which neither the amounts of eroded cover (at the surface or at unconformities) nor the geothermal gradients at the times of imprinting the ranks are known. If, however, the geothermal gradients within individual wells varied significantly with depth at the time of maximum burial, deviations from the relations shown on Fig. 5 would then result. Price (1991) cited sharp "dog-leg" bends, leading to approximately doubling of the geothermal gradients, in the coastal *Caillou Island* oilfield (a salt-ridge complex) and along the inland *Tuscaloosa* gas trend, both in southern Louisiana. For both examples, data from groups of wells were combined, and corrections to bottom-hole temperatures could not be well estimated. The *Caillou* example contrasts with the apparently uniform geothermal gradient in the *Point au Fer* well, also in coastal Louisiana, discussed above. Price (1991) correlated the bends in the geothermal gradients with "dog-leg" bends in the reflectance gradients. The reflectance data for the *Caillou* example, however, are quite inadequate to define a bend, and if a linear rather than log scale is used when plotting the reflectance data for the *Tuscaloosa* example, a curving bend in reflectance is seen to begin a kilometre higher in the well than the inferred sharp bend in geothermal gradient. Nevertheless, clear documentation of both temperatures and reflectance values in individual wells may show that sharp inflections of both parameters can be confidently correlated.

INFLECTIONS IN DEPTH/REFLECTANCE RELATIONS SHOWN BY OTHER WELLS

Although reflectance values extending to >1.5% have certainly been obtained for many wells, published data are rather few. Some of these wells have been discussed successively by different authors. As well as those discussed above, the most numerous group consists of those in areas where substantial but unknown amounts of erosion have

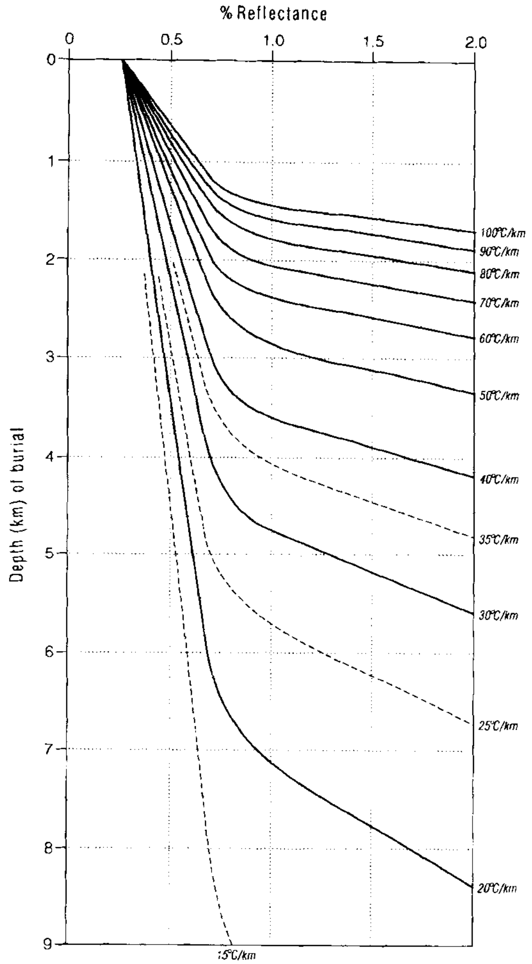

Fig. 5.Generalised depth/reflectance/geothermal gradient diagram, for which a surface temperature of 15°C and a surface reflectance value of 0.25% are accepted.

taken place, either at the present surface or at a subsequently buried unconformity. In the following examination of many available sets of well data, these data are plotted with a linear reflectance scale and depth/reflectance relations are then inferred and compared with the generalised depth/reflectance/geothermal gradient relations of Fig 5. Inferences of paleogeothermal gradients and maximum depths of burial are made for some of the wells.

***Panarctic Chads Creek B-64,* Melville Island, Arctic Canada** (Fig. 6)

Gentzis and Goodarzi (1990) used this well to illustrate the effect of a diabase sill, principally in the context of the reflectance of bitumen. Vitrinite reflectance values were also given, but only bitumen reflectance values adjacent to the sill itself. The heating affected only a small thickness of strata, and the well was drilled for 1.5 km below the sill, far below the effect of heating. Fig. 6A, plotted with a linear reflectance scale in place

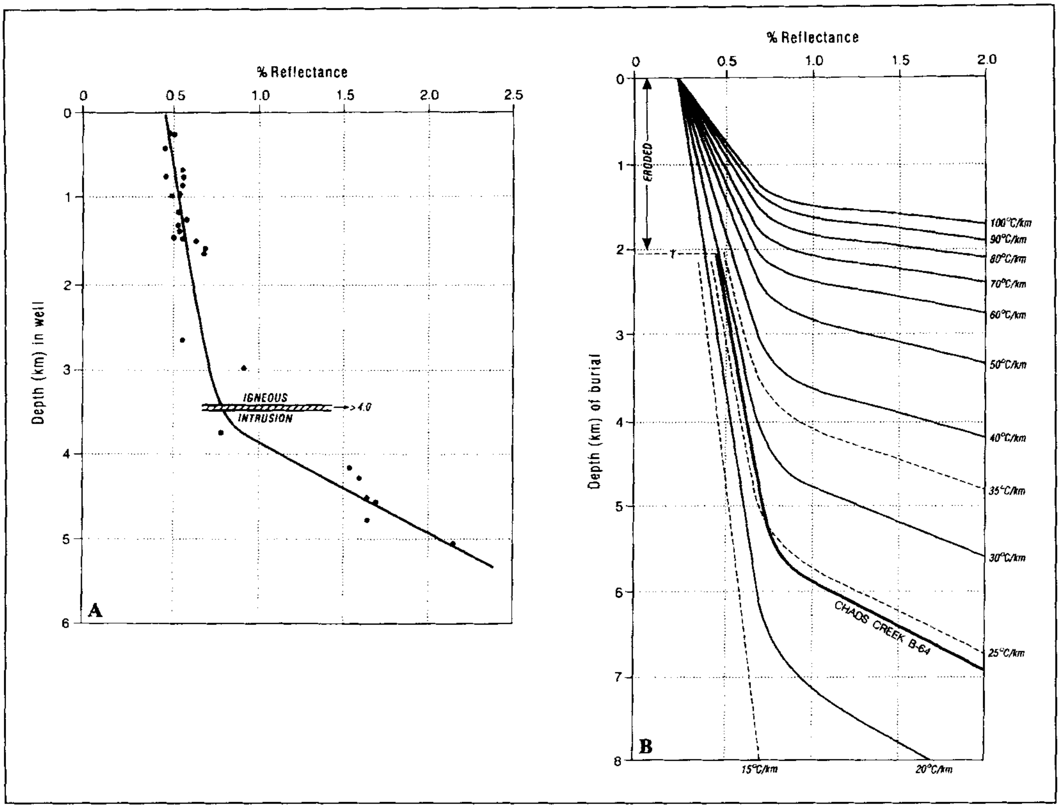

Fig. 6. *Panarctic Chads Creek B-64*, Arctic Canada.
A: Adopted depth/reflectance relation. B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well. Data from Gentzis and Goodarzi (1990).

of a log scale, shows the inferred depth/reflectance relation, apart from the sill-affected section. A clear inflection shows between 0.7% and 1% Ro, even though few data are available over this part of the range. Gentzis and Goodarzi (1990) did not interpret the well in terms of maximum depth of burial and paleogeothermal gradient.

For this well, as for others discussed below, it is possible to estimate the thickness of former deposits eroded from above the well sequence. The inferred reflectance/depth profile from Fig. 6A is plotted on the standard diagram, making a compromise between the slope of the low-rank gradient (which ideally projects to 0.25% Ro), the slope of the high-rank gradient, and the shape and position of the bend between the two gradients. The position of the top of the well is now fixed, and consequently so is the thickness of eroded sediments. Fig. 6B indicates that there has been c.2 km of erosion from above the Lower Cretaceous top of *Panarctic Chads Creek B-64*, and a paleogeothermal gradient of c.24°C/km.

Elmworth 6-28-68-13 WGM, Alberta Deep Basin, Canada (Fig. 7)

Welte *et al.* (1984) used the maturity profile of this well, together with the geological history, to estimate the progress of methane generation. A linear reflectance scale was used, as in Fig. 7. The shape of the depth/reflectance curve, which was not critical for their discussion, includes a marked inflection between 0.75% and 1% Ro, and provides a good fit on the standard diagram at a geothermal gradient of c.21°C/km. Nearly 5 km

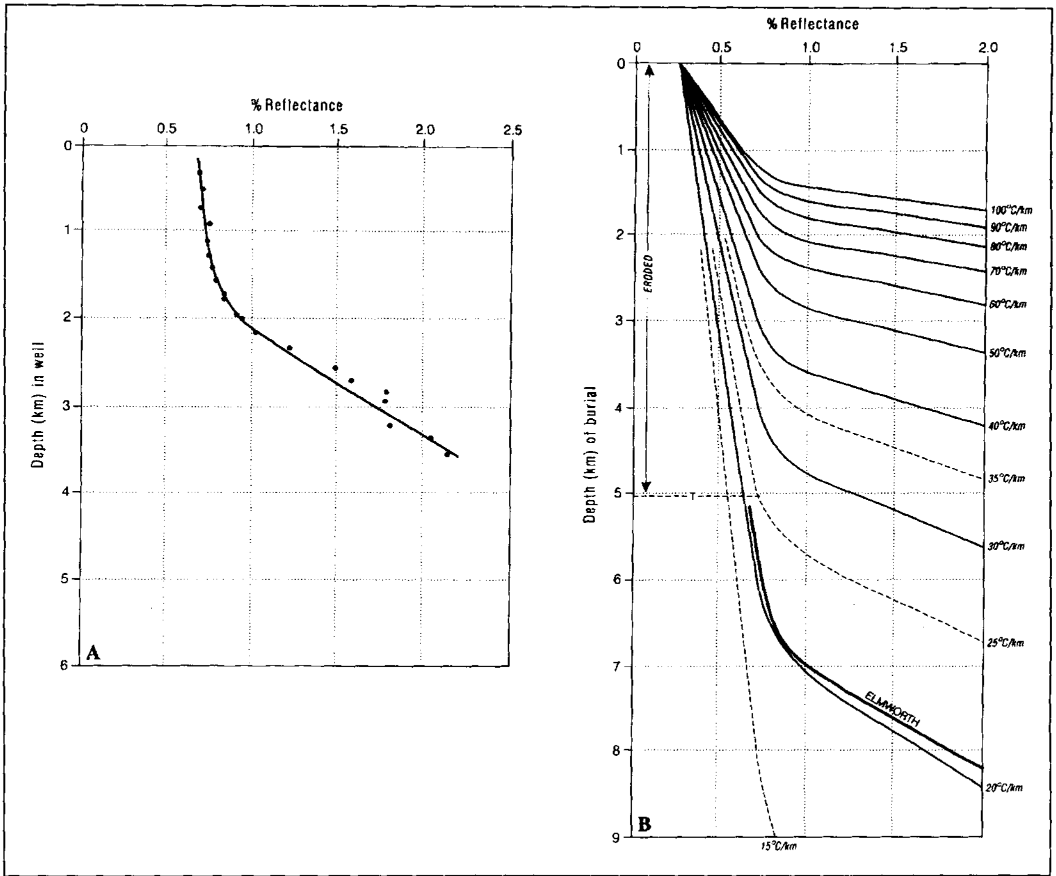

Fig. 7. *Elmsworth 6-28-68-13WGM*, Alberta Deep Basin, Canada.
A: Adopted depth/reflectance relation. B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well. Data from Welte *et al.* (1984).

are inferred to have been eroded from above the Upper Cretaceous rocks at the surface. Welte *et al.* (1984) estimated the erosion to be c.1.5 km, which would require a reflectance of 0.7% Ro to be attained at an improbably small depth of c.2 km.

Sable Sub-basin wells, Scotian Basin, offshore Nova Scotia, Canada (Fig. 8)

Reflectance data are available for several wells in the Sable Sub-basin, including *Alma F-67, Glenelg D-23, Venture B-52* and *South Venture O-59* with reflectance values extending higher than 1.25%. All the published depth/reflectance plots used a log scale for reflectance. The wells record an Early Jurassic to Recent sequence, with only slow subsidence in the Cenozoic. Data for these wells, plotted with a linear reflectance scale, are shown on Fig. 8A.

In the context of estimating overpressuring and hydrocarbon generation, Williamson (1995) used reflectance data from *Alma F-67* in calibrating models that included calculated reflectance values. *Glenelg J-48* was used as one example by Williamson and DesRoches (1993, p. 244) in presenting a maturation framework - "*models resulting from an examination of the interplay between the subsidence, compaction and thermal histories of 24 wells*"; thermal histories required the specification of heat flow and thermal conductivities. Mukhopadhyay *et al.* (1994) compared measured and calculated reflectances for *Venture B-52*,

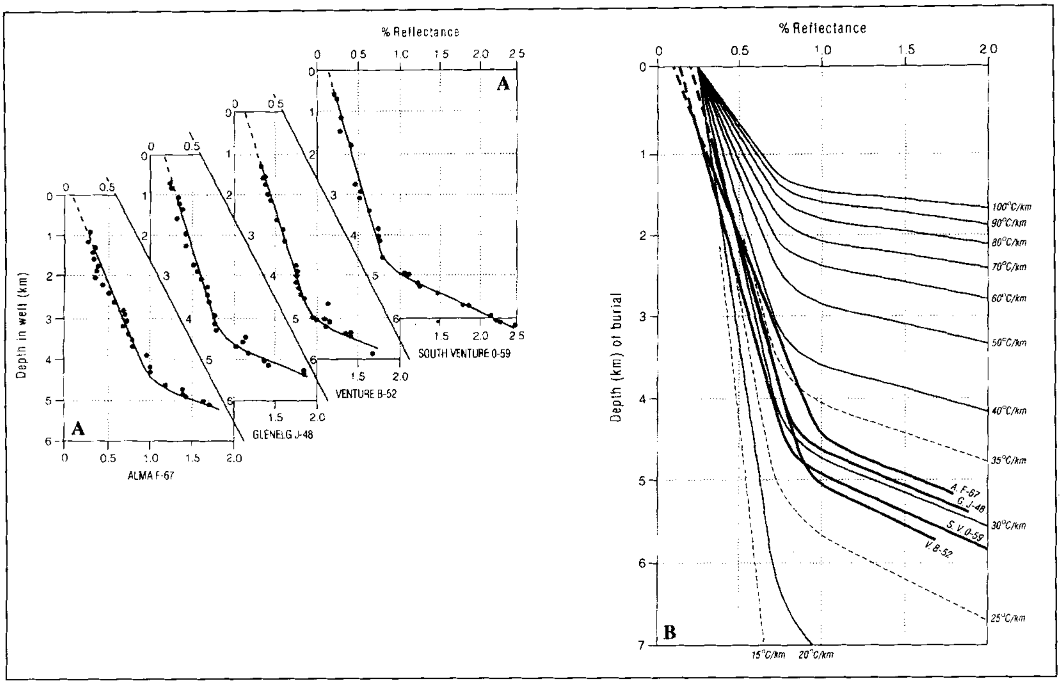

Fig. 8. Sable Sub-basin, Scotian Basin, offshore Nova Scotia.
A: Adopted depth/reflectance relations in *Alma F-67* (data from Williamson, 1995), *Glenelg J-48* (data from Williamson and DesRoches, 1993), *Venture B-52* (data from Mukhopadhyay *et al.*, 1994) and *South Venture O-59* (data from Mukhopadhyay and Wade, 1990).
B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. Wells are plotted as though they are at their present maximum depths of burial.

and, using both sets of results, estimated the timing of hydrocarbon maturation and migration; they used the EASY %Ro method of Sweeney and Burnham (1990) to obtain calculated reflectance values. Mukhopadhyay and Wade (1990) provided reflectance data for *South Venture O-59*, but were principally concerned with organic facies within the mature source rocks.

Except for *Alma F-67*, the wells show a clear inflection between c.0.7% and 1.0% Ro and the upper parts of the reflectance curves extrapolate to 0.2% Ro at the surface, consistent with a lack of erosion at the tops of the wells. Down to c.4.5 km, the reflectance profile in *Alma F-67*, and less prominently those in the other wells, is unusual in having sections of the well that show little increase in reflectance alternating apparently systematically with sections that show rather rapid increase. These fluctuations do not appear to correlate from well to well at formation boundaries, but are presumably related to variations in thermal conductivity controlled by lithology.

Temperature data for *Alma F-67* were given by Williamson (1995, fig. 7a), and a geothermal gradient map, using the deepest corrected bottom-hole temperatures (and 11.8°C for the sea bottom temperature), was given by Issler (1984, fig. 4). From these, the estimated geothermal gradients are: *Alma F-67* — 30°C/km; *Glenelg J-48* — 28°C /km; *Venture B-52* — 25.5°C/km; *South Venture O-59* — 26°C/km.

Fig. 8B shows the inferred depth/reflectance relations of the four wells plotted on the general diagram as though the wells were at their maximum depths of burial. Except that the minimum reflectances, extrapolated to the surface, are a little low, the depth/reflectance relations are generally consistent with the general pattern. The inferred geothermal

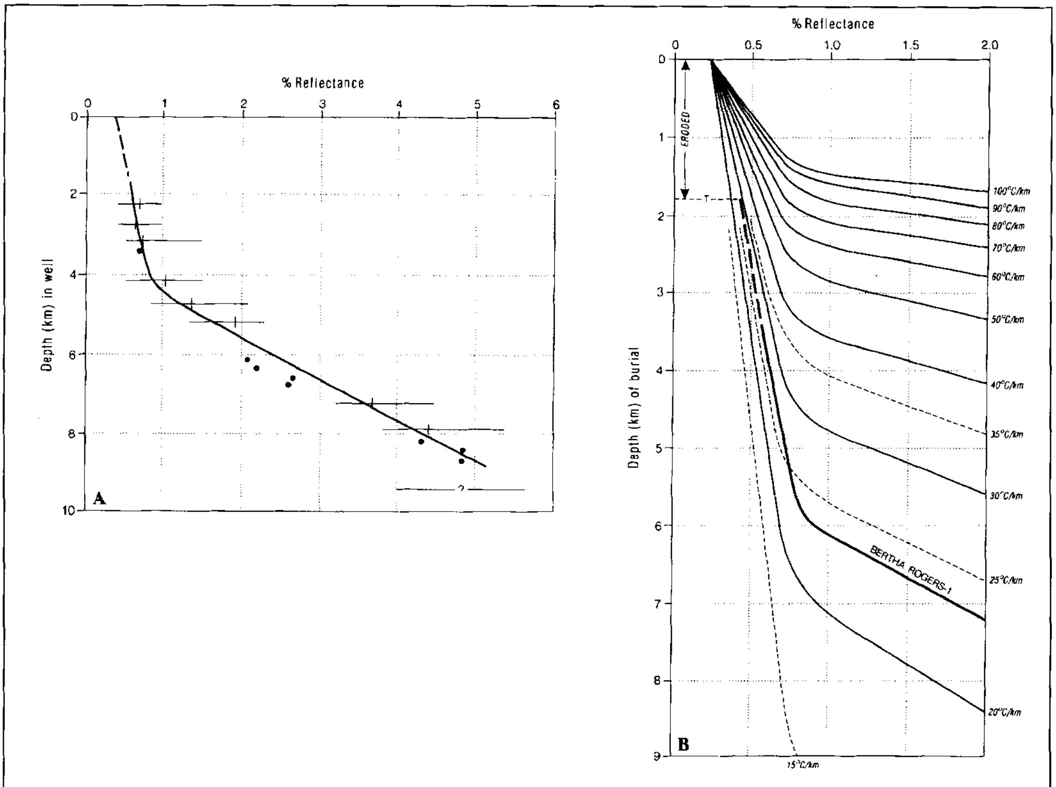

Fig. 9. *Bertha Rogers-1*, Oklahoma, USA.
A: Adopted depth/reflectance relation. B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well. Data from histograms of Price *et al.* (1981, with approximate mean reflectance values and ranges using only the best-defined histograms). Additional data (dots) from Price (1992).

gradients are, however, c.3°C/km lower than at present; at a depth of 5 km, roughly at 1% Ro, the estimated temperature differences are c.15°C. In the thermal modelling of *Alma F-67* (Williamson, 1995, fig. 7), *Glenelg J-48* (Williamson and DesRoches, 1993, fig. 6) and *Venture B-52* (Mukhopadhyay *et al.*, 1994, fig. 3), heat flow was accepted as declining progressively since deposition of the sequences began, and the decline may have resulted in declining geothermal gradients.

Bertha Rogers-1, Oklahoma, USA (Fig. 9)

The organic geochemistry of this well, which penetrated 9.6 km of Permian to Cambrian sedimentary rocks, was discussed by Price *et al.* (1981). Price (1992) provided additional reflectance data. Included in Price *et al.* (1981) were histograms of vitrinite reflectance, some of which were so wide — for example from 0.35 to 3.3% Ro at a depth of 8.3 km — that they cannot be used; Price *et al.* regarded the low reflectance values in this sample as "notable", but no explanation was offered. Those samples that can be regarded as having reasonably well-defined histograms, ignoring single values discrete from the majority, are shown on Fig. 9A. Particularly important are the six shallowest samples, for which the reflectance values were regarded by Price *et al.* as showing "tight distributions". These samples exemplify an inflection in the depth/reflectance relation in the 0.7% to 1.1% Ro range. As interpreted in Fig. 9B, the geothermal gradient at the time of maximum burial was c.24°C/km, and 1.7 km of the section has since been eroded.

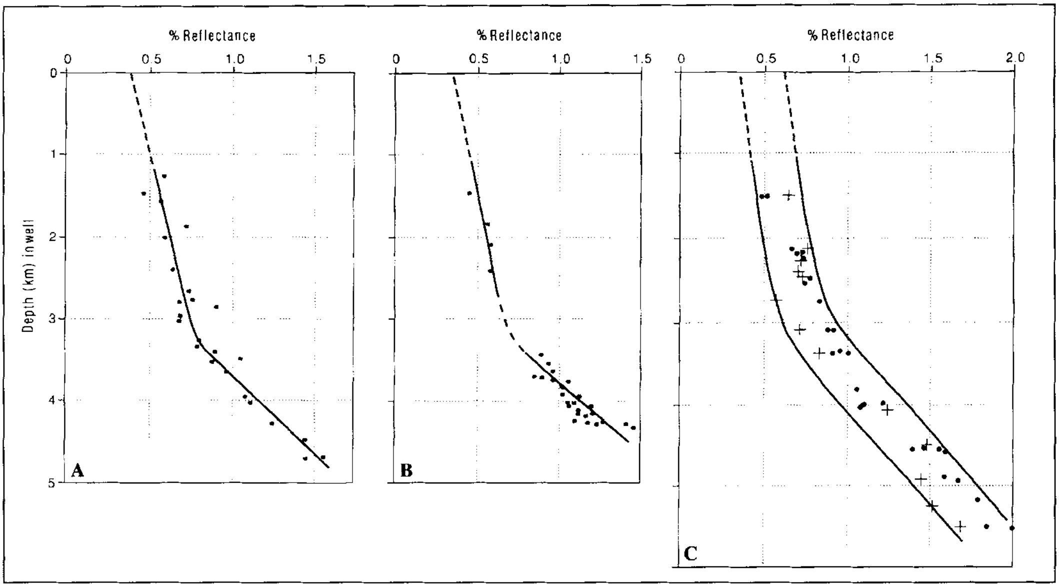

Fig. 10. Northern Green River Basin wells, Wyoming, USA: adopted depth/reflectance relations. A: *Rainbow 1-34 Pacific Creek* (data for cuttings samples from Law *et al.*, 1989, fig. 5). B: *Belco 3-28 Merna Unit* (data from Spencer, 1987); C: *El Paso Natural Gas Wagon Wheel-1* (data from Spencer, 1984 - dots, and from Pollastro and Barker, 1986 - crosses).

Northern Green River Basin wells, Wyoming, USA (Figs 10 and 11)

Several studies include reflectance data for wells in this area: for *Rainbow 1-34 Pacific Creek Federal* well, for *Belco 3-28 Merna Unit* well, and most notably for *El Paso Natural Gas Wagon Wheel-1*. The wells have early Cenozoic sediments at the surface.

For the Pacific Creek area, Law *et al.* (1989a) presented a depth/reflectance diagram on which the cuttings samples from *Rainbow 1-34 Pacific Creek Federal* well are separately distinguished; these are plotted on Fig. 10A. Combining these values with those from core samples from two wells, and using a log scale for reflectance, Law *et al.* (1989a) inferred two sharp inflections in the depth/reflectance relation, with a middle portion showing very little increase of reflectance, from 0.75-0.8% Ro, over a depth of c.0.5 km. While two samples are exceptional, Fig. 10A can be interpreted as showing a single inflection at 0.75% to 0.85% Ro.

Spencer (1987) presented a depth/reflectance diagram for the *Belco 3-28 Merna Unit* well, using a log scale for reflectance, in the context of discussing overpressuring and hydrocarbon generation in the wider Rocky Mountain region. Using a linear scale for reflectance, the data are presented on Fig. 10B. There are few data points with <0.6% Ro, and a gap of 1.5 km between these and numerous but rather scattered points with values between 0.85% and 1.5% Ro. Accordingly, the depth/reflectance curve in Fig. 10B is poorly controlled.

Initial data for *Wagon Wheel-1* were provided by Spencer (1984), in a discussion of overpressuring and hydrocarbon generation; additional data were given by Pollastro and Barker (1986), who used clay mineral, reflectance and fluid inclusion studies to infer a thermal and burial history for the Pinedale anticline. All the reflectance data are used in Fig. 10C. In illustrating the depth/reflectance relations, these authors all used a log scale for reflectance, as did Burnham and Sweeney (1989) when using *Wagon Wheel-1* to exemplify the comparison between observed reflectance values and those calculated

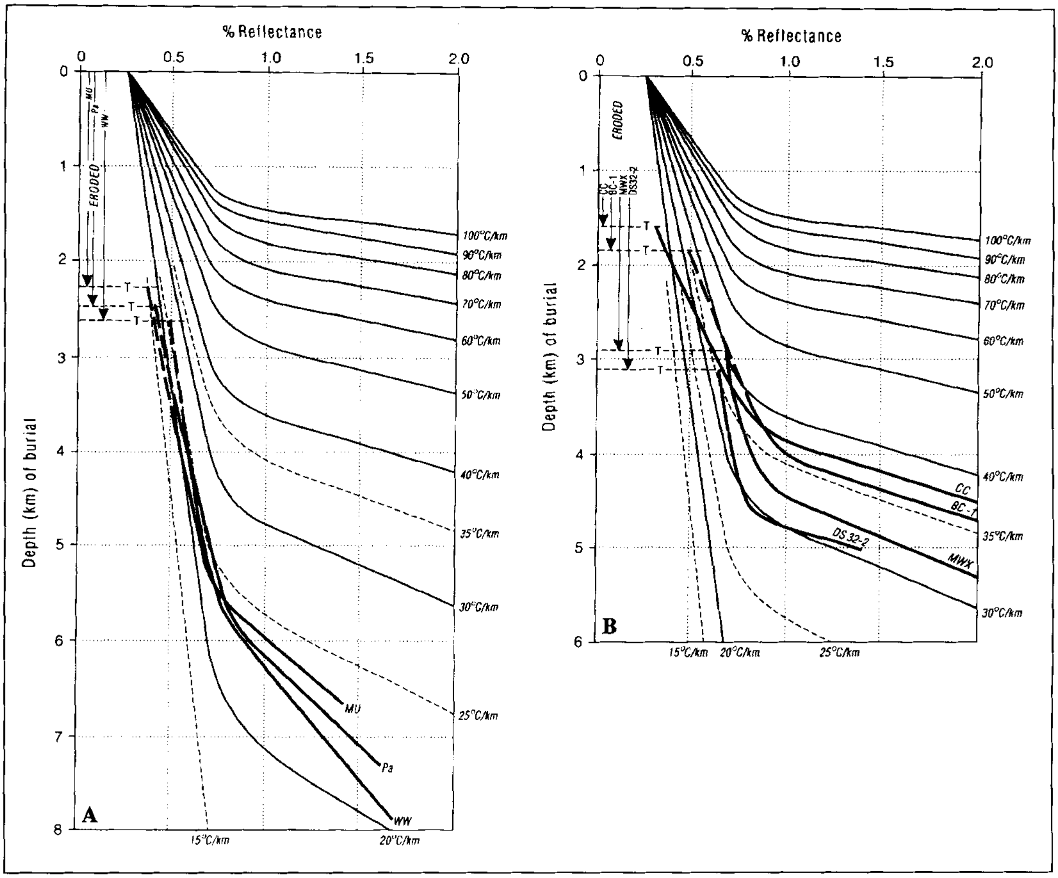

Fig. 11. Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well.
A: Northern Green River Basin wells; B: Piceance Basin wells.

using kinetic equations. Because of the different sets of data, a band rather than a line is drawn on Fig. 10C in inferring an inflection in the depth/reflectance relation in the 0.6% to 0.9% Ro range.

Fig. 11A shows inferred maximum depths of burial and paleogeothermal gradients for the three wells. For *Wagon Wheel-1*, the middle of the Fig. 10C band is used, but the fit on the standard diagram is not good; nor is it any better with either set of data separately. For this northern part of the Green River Basin, paleogeothermal gradients of 22-24°C/km are inferred, with thicknesses eroded of 2-3 km. Present geothermal gradients are higher: Spencer (1987, fig. 4) gave a gradient of 29°C/km for the *Merna Unit* well, and also (1987, fig. 8) an approximate corrected temperature at 3,170 m in *Wagon Wheel-1*, which gives a gradient of c.25°C/km. Assuming 20°C surface temperature at present and in the past, Fig. 11A indicates that 1.5% Ro was attained at a temperature of c. 177°C in these wells, whereas at present the temperatures are c.155°C in the *Merna Unit* well and c.140°C in *Wagon Wheel-1*. The temperature difference in *Wagon Wheel-1* is consistent with that inferred by Naeser (1986, p. 69) on the basis of a fission track study: "*a relatively rapid temperature decrease of 20°C or more*" in the last 2 to 4 million years. Pollastro and Barker (1986) inferred a paleogeothermal gradient of 24°C/km and an eroded thickness of 1.7 km.

Piceance Basin wells, Colorado, USA (Figs 11 and 12)

Several studies provide reflectance data for wells in this area, principally for the *MWX* site, but also for *GRS-REI-1 Deep Seam 32-2*, *Crystal Creek A-2*, *Sunlight Federal-2* and *Baldy Creek-1*.

The initial reflectance record for the *MWX site*, combined with that of a nearby Arco-Exxon well, was presented by Bostick and Freeman (1984), and *MWX* alone was shown by Spencer (1987) and by Nuccio and Johnson (1989). Their data, together with many additional reflectance values, were tabulated by Law *et al.* (1989a). Whereas all these authors used a log scale for reflectance, Fig. 12A, on which all the data are plotted, uses a linear scale. Bostick and Freeman (1984) used the reflectance in inferring that maximum paleotemperatures were attained during the time of maximum burial, from 40 to 10 million years ago, the duration of heating being important. Spencer (1987) discussed the development of overpressuring in the context of this burial history, and Nuccio and Johnson (1989) used the *MWX* site wells as one example in considering hydrocarbon generation in relation to the development of maturity. Law *et al.* (1989a) accepted the reflectance profile in the *MWX* wells as "kinky", with little or no increase of reflectance over a depth of 0.5 km at c.0.9% Ro. Fig. 12A, however, shows that there are such large differences of reflectance between close-spaced samples that the drawing of particular kinks in the depth/reflectance relation is not warranted; the inferred relation, with an inflection between 0.8% and 1.0% Ro is considered more probable.

Law *et al.* (1989b) inferred that the depth/reflectance profile in the *GRI-REI-1 Deep Seam 32-2* well could be interpreted by three segments. A shallow (Early Cenozoic) segment had 0.9% Ro at its base, yet the top of the middle segment showed only 0.65% Ro - a scarcely possible situation. Reflectance in the bottom segment increased rapidly with depth compared with the middle one, and Law *et al.* (1989b, p. 341) concluded that "*perturbations in the paleothermal gradient*" associated with a "*history of abnormally high pore pressure*" were the cause of the segmented depth/reflectance profile. Fig. 12B, using a linear scale for reflectance, interprets the data as including a few exceptional reflectance values in the context of a single curve with an inflection between 0.8% and 1.0% Ro.

Of the three further depth/reflectance profiles from the Piceance Basin figured by Nuccio and Johnson (1989), *Crystal Creek A-2* (Fig. 12C) and *Baldy Creek-1* (Fig. 12D) show inflections between 0.75% and 1.0% Ro; *Sunlight Federal-2* extends to only 0.8% Ro.

Shown in relation to the generalised depth/reflectance diagram (Fig. 11B), the Piceance Basin wells indicate a range of paleogeothermal gradients between 30°C/km and 38°C/km, with eroded thicknesses of between 1.5 and 3 km. *Crystal Creek A-2* fits least well, although the gradient below the inflection is similar to those of the other wells. The paleogeothermal gradient at the *MWX* site is similar to that inferred by Bostick and Freeman (1984), but the inferred thickness eroded is greater - 2.9 km compared with Bostick and Freeman's 1.4 km; 1.4 km would not lead to 0.6% Ro at a depth of 1.4 km without a much higher geothermal gradient.

Regardless of the degree of success in matching depth/reflectance gradients with the standard diagram, both the Piceance Basin wells and the Northern Green River Basin wells show inflections between roughly 0.7% and 1.0% Ro. A major contrast, however, shows (Fig. 11) between these two groups, with the Piceance Basin wells indicative of markedly higher paleogeothermal gradients than the Northern Green River Basin wells.

"Closely-spaced wells", Maracaibo Basin, Venezuela (Fig. 13)

Sweeney *et al.* (1990), in discussing oil generation in the Maracaibo Basin, used data from many wells interpreting their thermal histories. Fig. 13B shows their depth/reflectance diagram for "closely-spaced wells", with "*a jog in the data caused by the higher geothermal*

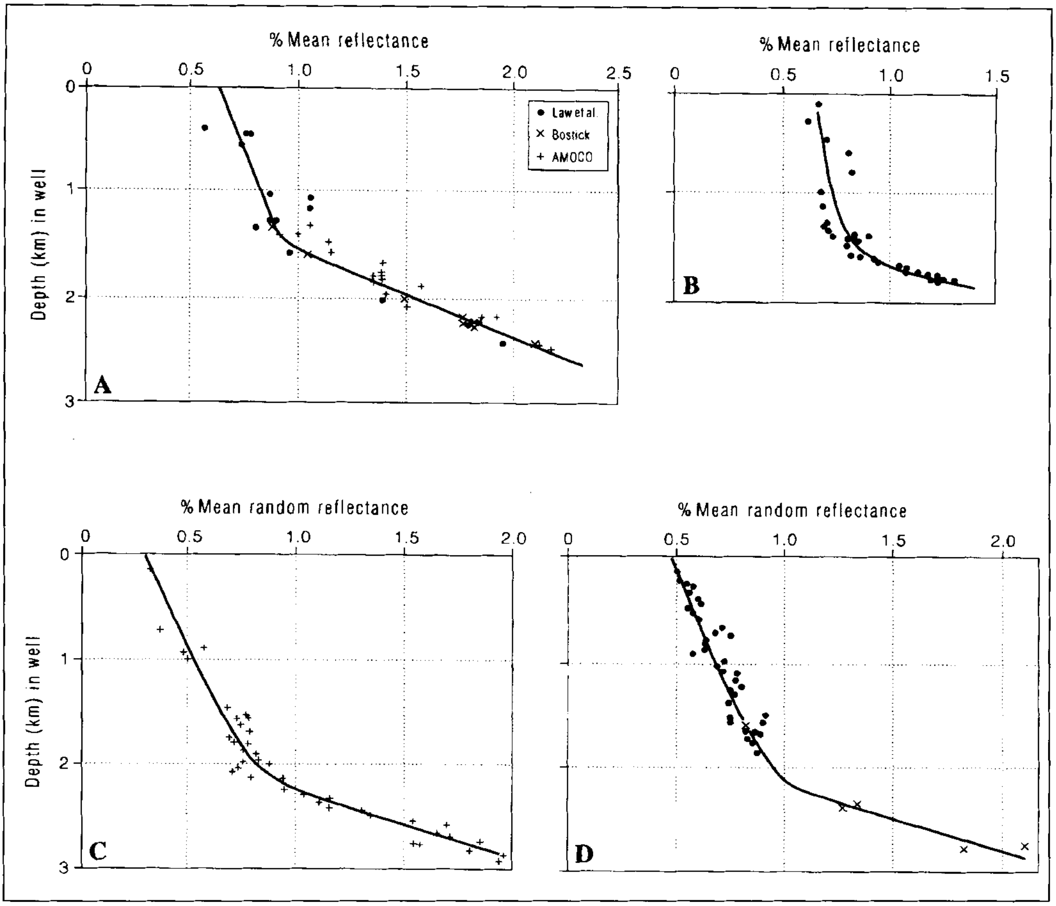

Fig. 12. Piceance Basin wells, Colorado, USA: adopted depth/reflectance relations.
A: *MWX* site (data from Law *et al.*, 1989a, table 1).
B: *GRS-REI-1 Deep Seam 32-2* (data from Law *et al.*, 1989b);
C: *Crystal Creek A-2* (data from Nuccio and Johnson, 1989);
D: *Sunlight Federal-2* — dots; *Baldy Creek-1* — crosses (data from Nuccio and Johnson, 1989).

gradient below the Colon shale". Sweeney *et al.*, however, did not place these wells in the context of their subsequent subdivision of the basin into areas with different thermal histories; nor did they detail the stratigraphy. The lower parts of the wells are in Cretaceous-Eocene formations, and Sweeney *et al.* emphasised the "*large uncertainty in the amount of post-Eocene and post-Miocene erosion*". From the presence of overpressuring and the implication that part of the sequence is Miocene, it is apparent that the wells are located in the area where oil generation was inferred to have started in the Eocene, to have stopped because of post-Eocene erosion, and then to have resumed in the Neogene following Miocene and later deposition.

Fig. 13A shows the data plotted with a linear scale for reflectance. The interpretation shows a typical inflection between 0.8% and 1% Ro, and the slopes of the segments above and below the inflection do not greatly differ from those which might be expected with the inferred geothermal gradient of 37°C/km. The latest Cretaceous La Luna Formation, the principal source rock, would have been at a depth of c.4.2 km, with a reflectance of

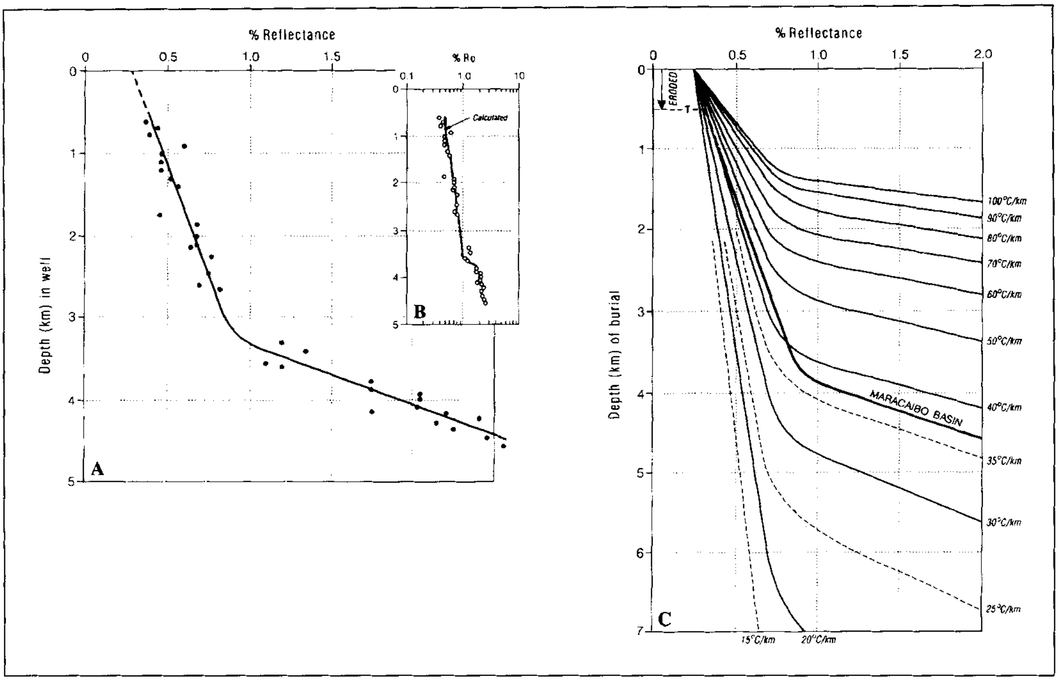

Fig. 13. "Closely-spaced wells", Maracaibo Basin, Venezuela.
A: Adopted depth/reflectance relation. B: Data and calculated depth/reflectance relation of Sweeney *et al.* (1989). C: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well.

c.2.0%, having passed through the "oil window". Only 0.5 km of post-Eocene erosion would be required (Fig. 13C), perhaps insufficient to stop oil generation unless the geothermal gradient was reduced. The effect of additional Neogene sedimentation on oil generation would have depended on the geothermal gradient, probably much lower in the Neogene rocks than in the Eocene since Talukdar *et al.* (1986) reported a present-day average geothermal gradient of only 22°C/km in Tertiary rocks of the Maracaibo Basin. Sweeney *et al.* (1990) did not report the present-day geothermal gradient in the closely-spaced wells that they exemplified.

Logbaba well, Cameroon (Fig. 14)

Tissot and Espitalié (1975) developed a model of the thermal degradation of organic matter, which they used in conjunction with vitrinite reflectance values to estimate paleogeothermal gradients. They concluded (p. 743) that "*a vitrinite evolution model can be used in most cases to reestablish the thermal history of the organic matter*". As an example, they studied the *Logbaba* well, showing 17 reflectance values. They assumed a paleogeothermal gradient of 50°C/km for the well.

Alpern *et al.* (1978), in the context of a study of the effects of artificial heating on organic matter, listed 24 vitrinite reflectance values for the *Logbaba* well, apparently including those used by Tissot and Espitalié (1975). These are plotted on Fig. 14A, on which an inflection in the depth/reflectance relation is shown between 0.6% and 0.9% Ro, at slightly lower values than in most other sequences. A paleogeothermal gradient of 40-45°C/km is inferred on Fig. 14B, considerably lower than that used by Tissot and Espitalié (1975). A thickness of c.0.8 km is estimated to have been eroded from above the Cretaceous-Paleocene sequence drilled in the well.

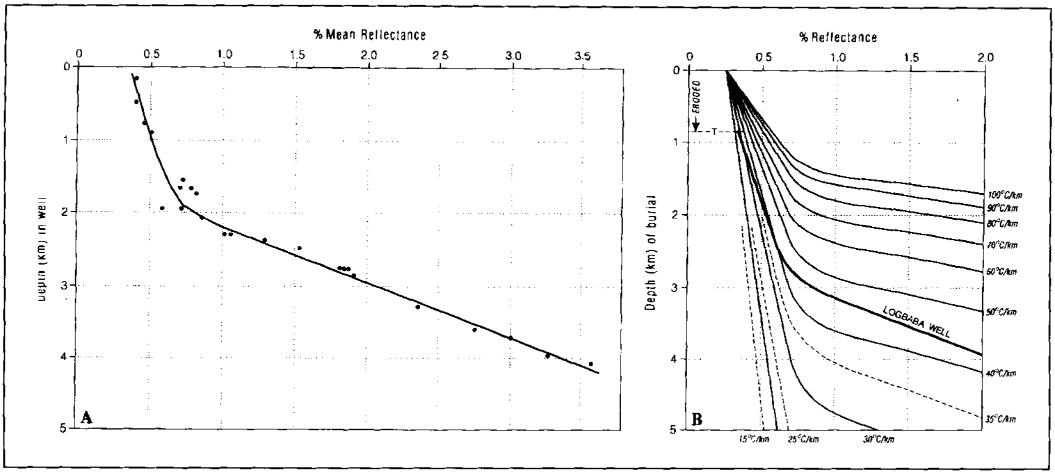

Fig. 14. *Logbaba* well, Cameroon.
A: Adopted depth/reflectance relation. B. Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well. Data from Alpern *et al.* (1978).

Gironville **well, France** (Fig. 15)

The variations of reflectance in the Carboniferous strata of this well, situated c.80 km SW of the Lorraine coal basin, were initially examined by Alpern (1966), who presented two sets of data: plotted ranges of reflectance in >70 samples in his fig. 5 and a list of 24 mean values in his table 1. The approximate envelope of the larger set (Fig. 15A) includes most individual points for the smaller set. Alpern drew attention to an increasing rate of increase of reflectance with depth. The highest coals examined from the *Gironville* well have a reflectance of c.0.75%, whereas in the mined area to the NE, Alpern showed that coals at a similar stratigraphic position have a reflectance of c.1.0%; he noted that the apparent rate of increase with depth in the higher strata is particularly low in comparison with that in the strata drilled at *Gironville.*

Rouzaud *et al.* (1991) used various techniques on *Gironville* samples to characterize the structural changes during progressive coalification, and showed a depth/reflectance relation based on these samples, which had unfortunately been oxidised in storage. The reflectance values shown on Fig. 15A are from numerical data provided by Dr J. N. Rouzaud (*pers. comm.*, 1993). With few exceptions, the data correspond closely with those of Alpern (1966); a notably low reflectance (and low carbon) sample from 2,440 m probably represents cavings as it falls at the base of the zone of samples contaminated by cavings noted by Alpern (1966). Durand *et al.* (1986) presented a small number of reflectance values for the *Gironville* well, but they are systematically lower than those of both Alpern (1966) and Rouzaud (*pers. comm.*), and are not reproduced here. Both Alpern (1966) and Rouzaud *et al.* (1991) used linear scales for reflectance.

The *Gironville* data show an inflection close to 1.0% Ro, but the slope of the lower-rank part of the depth/reflectance relation is not well defined. In keeping with the values in Alpern's Table 1 and those of Rouzaud (*pers. comm.*), a reflectance of 1.0% Ro is inferred at 2,200 m, and a smoothed gradient is accepted between 1.0% and 3.0% Ro, rather than the kink in the depth/reflectance gradient shown by the larger set of Alpern's data. A minor inflection at c.3.0% Ro is beyond the range considered in detail here. Transferred to Fig. 15B, the depth/reflectance relation is inferred to result from a geothermal gradient of c.32°C/km, with c.2 km eroded from above the top of the Carboniferous in the well. The overlying 1.1 km of Mesozoic has been reduced by erosion from a maximum

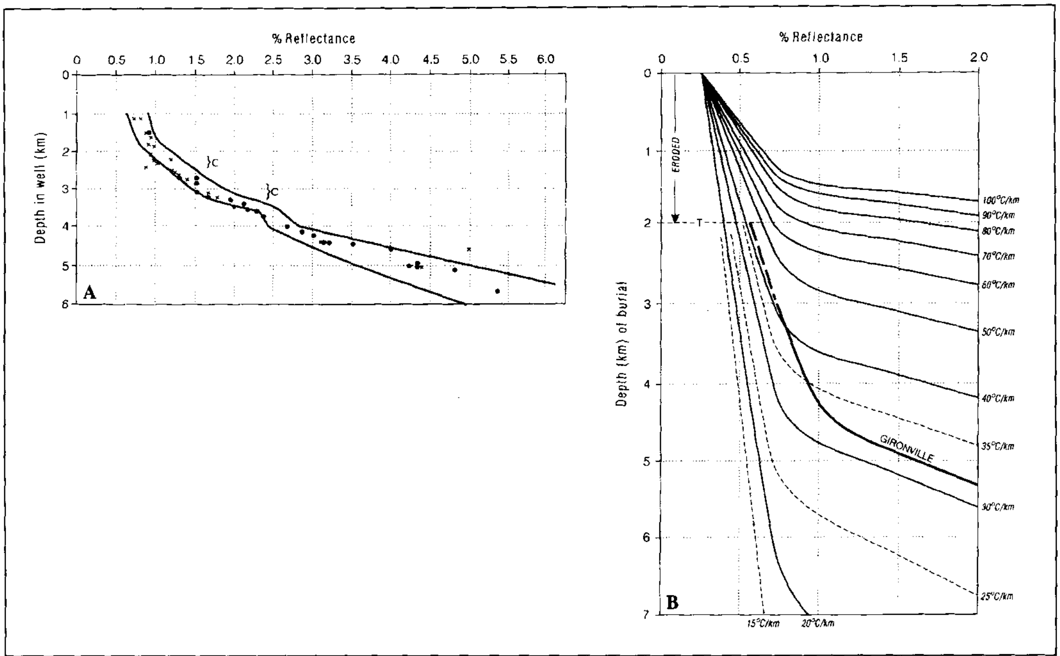

Fig. 15. *Gironville* well, France.
A: Depth/reflectance relations based on (a) data from Alpern (1966) (band is the approximate envelope of data in his fig 11; dots are from his table 1). (b) from Rouzaud (*pers. comm.*, 1993) (crosses); c = zones with samples contaminated by cavings (Alpern, 1966).
B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well.

of 1.5 km (Ungerer *et al.*, 1986). Accordingly the eroded c.2 km is likely to have been late Carboniferous. Alpern (1966, fig. 3) showed the Lorraine coal basin to include >3 km of Carboniferous strata younger than the *Gironville* sequence.

Ungerer *et al.* (1986) discussed the *Gironville* well as one example in attempting to use kinetic models for estimating paleotemperatures, with an emphasis on the increase of Tmax with depth. Their preferred paleogeothermal gradient was 40°C/km, with 1.5-2.0 km of erosion after the deposition of the highest Carboniferous strata in the well. They accepted that these figures "suffer great uncertainties".

Well *A*, North Sea (Fig. 16)

Wei *et al.* (1994) cited this well in using kinetic models of vitrinite reflectance in the context of reconstructing paleoheat flux; few details were given of the well, but their fig. 8 implies continuous subsidence to the present day, mainly through the Late Cretaceous and Cenozoic, and a temperature for the lowest vitrinite reflectance sample at 4.4 km of c.140°C. Fig. 16A shows the reflectance values taken from their fig. 7, which used a linear scale for reflectance, together with their inferred depth/reflectance relation, which cannot be extrapolated to a reasonable surface value; Fig. 16A also shows the now-preferred relation.

The preferred relation shows an inflection between Ro 0.65% and Ro 0.8%, but this is inadequately controlled because the highest reflectance value is only 0.88%; the relation has been fitted on the Fig. 5 generalisation (Fig. 16B) accepting that the well depths represent burial depths. The depth/reflectance relation is interpreted as resulting

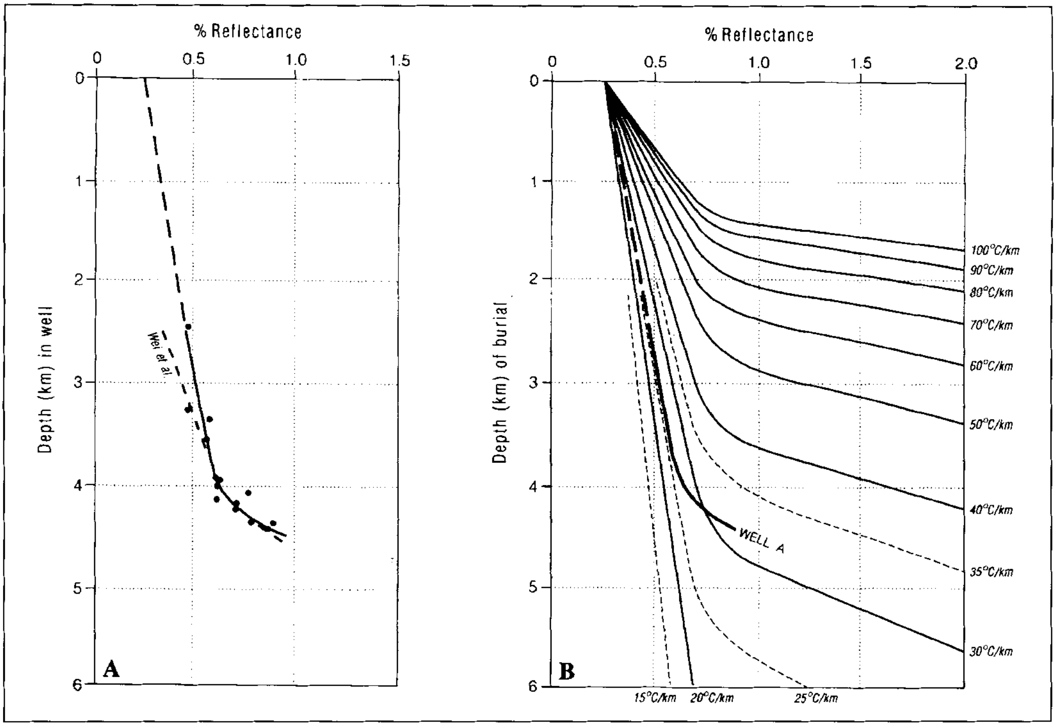

Fig. 16. Well *A*, North Sea.
A: Adopted depth/reflectance relation, and that of Wei *et al.* (1994).
B. Inferred relations of reflectance to maximum depth of burial and geothermal gradient.
T = Top of well. Data from Wei *et al.* (1994).

from a geothermal gradient of 27-30°C. The inferred temperature at 4.4 km is 125-145°C, closely similar to the apparent temperature at that depth. This is consistent with the statement by Wei *et al.* (1994, p. 275) that *"present-day heat flow is more important in determining the maturity than paleoheat flow"*.

DIO Baryulah-1, Nappamerri Trough, Eromanga Basin, Australia (Fig. 17)

Beeston (1995, fig. 11) presented reflectance data points and a depth/reflectance profile for this well, using a linear scale for reflectance. It penetrated a Mesozoic sequence ending with the mid-Cretaceous Winton Formation, which records the transition from a marine to a non-marine depositional environment, and is the youngest unit preserved in the basin (Goscombe and Coxhead, 1995). The adopted depth/reflectance relation (Fig. 17A) shows a clear inflection between 0.65% and 1% Ro, and is interpreted (Fig. 17B) as indicating a paleogeothermal gradient of 50-60°C/km, with erosion of c. 250 m.

Wells discussed by Dow (1977) (Fig. 18)

Dow (1977) presented depth/reflectance plots for "a typical Louisiana Gulf Coast well", "an Indonesian well" and "a Texas Gulf Coast well". The Louisiana well was stated to be in a continuously subsiding basin, and the others were inferred from the near-surface reflectance values to be in subsiding basins. Fig. 18 shows the data replotted using linear scales for reflectance, together with inferred depth/reflectance relations. Compared with almost all wells discussed above, and with the generalised diagram (Fig. 5), these wells show low extrapolated reflectance values at the surface: < 0.1-0.15% Ro,

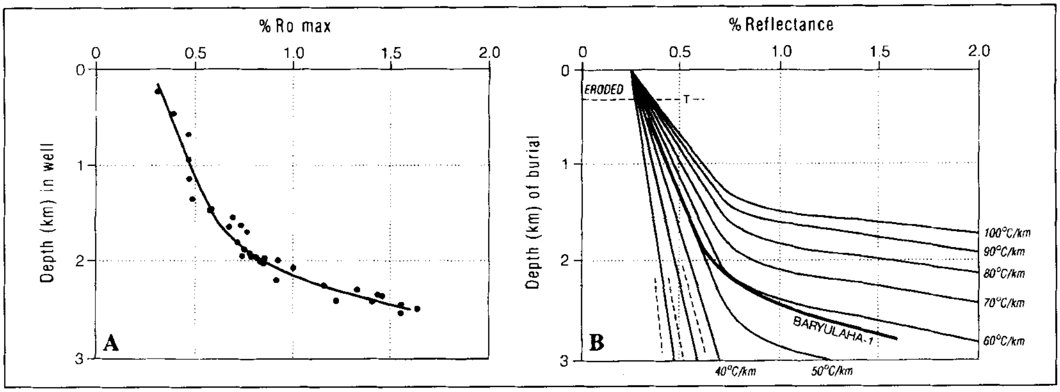

Fig. 17. *DIO Baryulah-1* well, Nappamerri Trough, Australia.
A: Adopted depth/reflectance relation. B: Inferred relations of reflectance to maximum depth of burial and paleogeothermal gradient. T = Top of well. Data from Beeston (1995, fig. 11).

c.0.1% Ro less than might be expected. Comparably, the inflections in the depth/reflectance relations are at c.0.6% Ro, substantially lower than might be expected. Because of these apparently low reflectance values, these wells were not used in constructing the depth/reflectance diagram (Fig. 5).

The Louisiana well (Fig. 18A) contrasts greatly with the *Point-au-Fer* well (Fig. 1B), also in Louisiana, and the lack of reflectance data from 2,900 m to 4,200 m detracts from the value of the sequence. Sweeney and Burnham (1990), in presenting their EASY %Ro model, used the Louisiana well, attributing a data set to Dow (1977).

The Indonesian well (Fig. 18B) was used by Dow (1977) to interpret an unconformity at a depth of c. 3,650 m as resulting from c.0.5 km of erosion of the underlying sequence. This interpretation involved the assumption that the inferred reflectance value at the base of the overlying Tertiary sequence (0.64% Ro) could be simply subtracted from that at the top of the Mesozoic (0.96%) to give the reflectance (0.32% Ro) at the top of the Mesozoic at the beginning of Tertiary sedimentation. If the reflectance at the base of the Tertiary is actually lower than that of the underlying Mesozoic, it can tell nothing about the reflectance and depositional history of the Mesozoic as the reflectance in the Mesozoic will not have increased as a result of Tertiary sedimentation. Accepting (Fig. 18B) a single depth/reflectance relation with a major inflection, it seems probable that the reflectance at the top of the Mesozoic at the unconformity was less after erosion than was attained later under the Tertiary cover, and that the reflectance values throughout the well were set under the maximum thickness of Tertiary sediments.

The Texas well was used by Dow to show the difference in reflectance between primary and recycled organic matter. Only the values for primary organic matter are used on Fig. 18C. The extrapolated Ro value of 0.1% at the surface contrasts markedly with 0.25% of *Cost-1* (Fig. 1D). There is an apparent inflection, but there are few data points below it.

GENERAL INFERENCES FROM THE WELL DATA

In addition to the wells taken for calibration of the general relations between vitrinite reflectance, depth of burial and geothermal gradient, the offshore Nova Scotia wells (Fig. 8) are also from a basin that may not have been inverted. As a group, these wells show a good fit to the generalisation in Fig. 5 and the approximate geothermal gradients. Well *A* (North Sea) (Fig. 16) may also be at its maximum depth of burial, and its depth/reflectance profile is also generally consistent with the relations shown on Fig. 5.

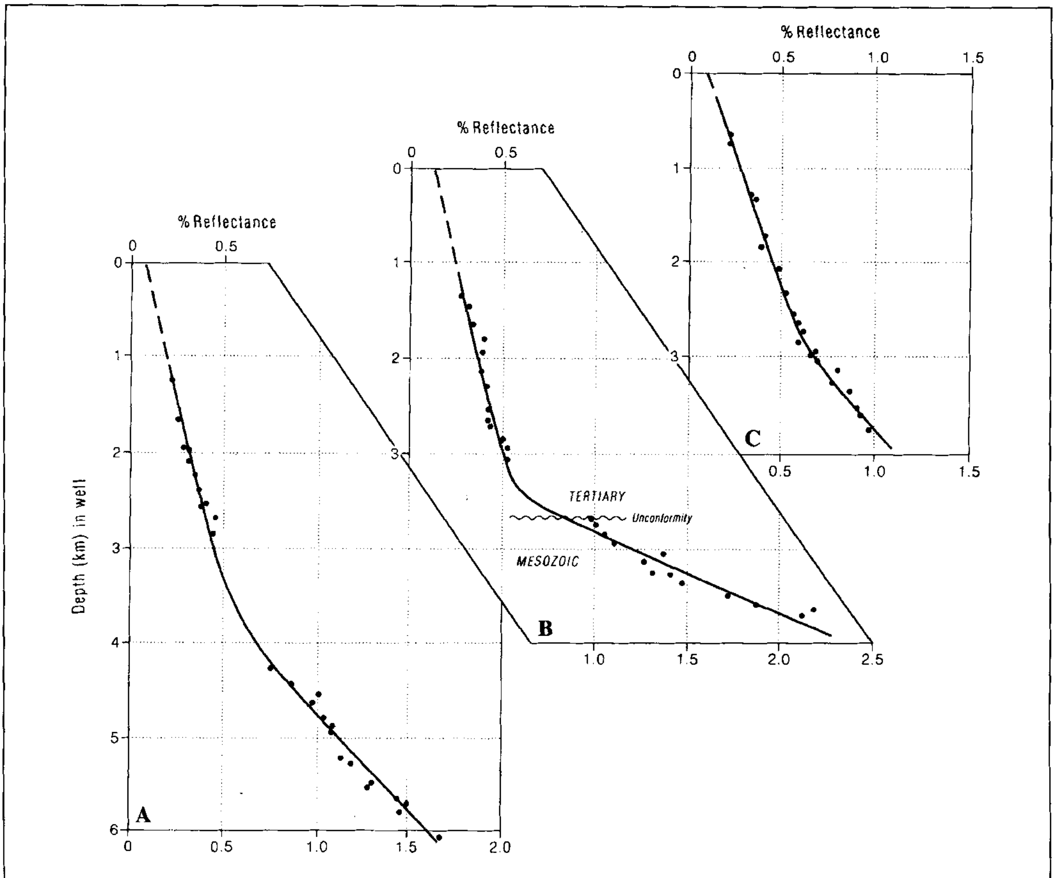

Fig. 18. Wells discussed by Dow (1977): adopted depth/reflectance relations. A: "A typical Louisiana Gulf Coast well". B: "An Indonesian well". C: "A Texas Gulf Coast well".

Only small thicknesses are inferred to have been eroded from *DIO Baryulah-1* (Fig. 17), the *Logbaba* well (Fig. 14) and "closely-spaced wells" in the Maracaibo Basin (Fig. 13), all of which have undergone uplift, probably in the mid-Cretaceous, Early Cenozoic and Late Cenozoic, respectively. These wells provide depth/reflectance profiles that are broadly consistent with Fig. 5, but the paleogeothermal gradients cannot be checked. Somewhat more problematic, because of greater and/or older eroded sections above the ground surface, are the remaining wells. Some of these show depth/reflectance profiles that fit the Fig. 5 generalisation well, for example, *Panarctic Chads Creek B-64* (Fig. 6) with Lower Cretaceous at the top, and *Elmworth 6-28-68-13 WGM* (Fig. 7) with Upper Cretaceous at the top. Others, such as those from the Northern Green River and Piceance Basins (Figs. 10-12) fit only moderately well (Fig. 5), but indicate consistent differences between these adjacent basins.

The widely-scattered data sources for the many wells discussed do not provide a confidently homogeneous set of data. In particular, the problems of comparability of reflectance measurements, and the inadequate numbers of measurements for some wells or sections of wells, may account for some depth/reflectance profiles being poor fits on Fig. 5. Nevertheless, in any interpretation of these profiles, the high probability of an inflection between differing upper and lower linear gradients should be anticipated.

THE IMPORTANCE OF THE INFLECTION BETWEEN 0.7% AND 1.0% Ro

In generalising the depth/reflectance relations for the many wells cited, some individual samples plot at considerable distances to one side of an adopted relation, usually balanced by other samples on the other side. The wide range of possible uncertainties affecting reflectance data, noted in the Introduction, makes this unsurprising, and some authors appear to have placed too much weight on a few samples in adopting particular shapes for the depth/reflectance relations. Indeed, Sweeney *et al.* (1990, p. 191) (see Fig. 13B) noted *"in some cases the thermal histories had to be adjusted to fit specific %Ro profiles or values"*. All the wells cited are interpreted as showing a single important inflection between 0.7% (rarely 0.6%) Ro and 1% Ro, with straight segments above and below.

The general shape of the depth/reflectance relations tends to be obscured by the use of a log scale for reflectance, and has unduly influenced some authors (e.g. Dow, 1977) to infer that the general relation, where the thermal history is simple, will be a straight line on a semi-log plot. Taking account of the normality of an inflection that is most prominent between 0.7% and 1.0% Ro is much more important than regarding individual samples or profiles as being critical to an inferred thermal history. The assumption that the depth/reflectance relation is best illustrated on a semi-log diagram in testing reflectance values calculated from kinetic equations against well data (cf. Burnham and Sweeney, 1989; Sweeney and Burnham, 1990) may well introduce an unwarranted problem, and may possibly lead to incorrect kinetic inferences.

A principal input into determining the thermal history, where erosion of the critical sequence has taken place either at an unconformity or at the present surface, is the amount of that erosion. Using the generalised diagram relating depth, reflectance and geothermal gradient (Fig. 5), notably different estimates are made for some wells than have previously been suggested. An important difficulty with erosion estimates based on stratigraphy is that erosion of the latest part of a depositional sequence — usually composed of unconsolidated sand and mud — is exceptionally easy; this part is rarely preserved, except in a still-subsiding basin. Further, rapid lateral changes of thickness commonly cannot be ruled out, causing problems in extrapolating from outcrop to substantial distances. The use of Fig. 5 depends on the imprinting of reflectances at the culmination of a single depositional episode, which may override an earlier episode in which the burial thickness or geothermal gradient, or both, resulted in a lower-rank sequence. It also assumes that the effect of time is insignificant once reflectances have been set at the maximum temperatures attained in a single depositional episode.

THE INFLECTION IN RELATION TO OIL GENERATION

Burnham and Sweeney (1989, fig. 14 and discussion) showed oil generation from vitrinite to be incipient at 0.6% Ro, at its fastest between 0.7% and 1.0% Ro, and tailing off to end at 1.2% Ro. It is no coincidence that the depth/reflectance relation should change its character as a result of oil generation. The chemistry of the coal or coaly particles changes dramatically — as seen, for example, on a van Krevelen diagram where the rank increase in bituminous coals is accompanied by a decline in H/C after a progressive rise through the pre-mature (lignite and sub-bituminous) stage of coalification. The coking properties of coal increase rapidly over the 0.55% to 1.0% Ro range, but the increase tails off to a maximum at c. 1.4% Ro, before rapidly declining (cf. Suggate and Boudou, 1993). Some oil generation is likely to continue through the whole range from 0.55% to 1.4% Ro, and perhaps further to the point of elimination of coking properties at c. 2.5% Ro. Price (1991) inferred that it continued to 2% Ro.

In a discussion of the relationships between aromaticity, vitrinite reflectance and maceral composition of coals, Carr and Williamson (1990, fig. 4) showed an abrupt inflection in the relation between aromaticity and reflectance at 0.7% Ro in vitrains and

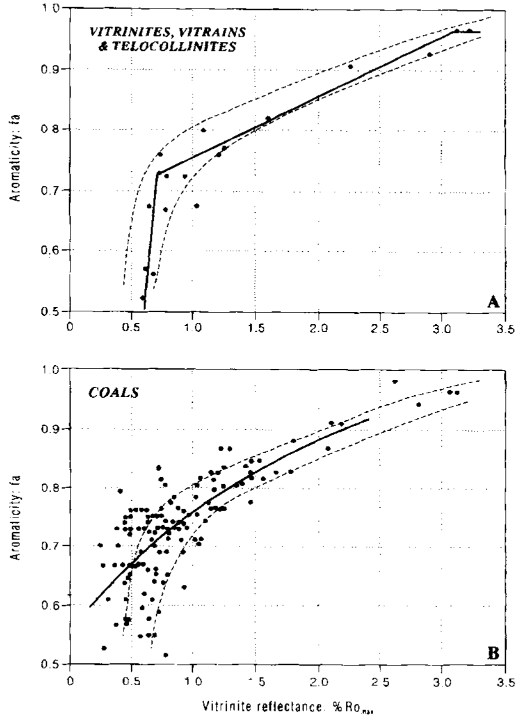

Fig. 19. Relations between reflectance and aromaticity; data from Carr and Williamson (1990, figs. 1 and 4). A: Vitrinites, vitrains and telocollinites; the full line is the generalization of Carr and Williamson, and the dashed band is the preferred relation; B: Coals; full line is the relation of Carr and Williamson, and the dashed band is transferred from A.

vitrinite, but their data points would be better generalised by a rapid but progressive change between 0.7% and 1.0% Ro (Fig. 19A). This generalisation then applies somewhat better (Fig. 19B) to the coals illustrated in their fig, 1 than does the polynomial function illustrated in their fig. 2. Their discussion centred on three stages in the developing relation between *fa* (aromaticity) and Ro (reflectance): an initial stage of the removal of non-aromatic carbons, in which *fa* increases without significant increase in Ro; a second stage, with the formation of multi-ring structural aromatic units with increases of both *fa* and Ro; and a third stage, in which reorganisation into large aromatic sheets leads to little increase in *fa* with progressive increase in Ro. Carr and Williamson recognised that the processes overlapped during maturation; however, the predominant influences at the three different stages show on Fig. 19 with the recognition of a marked inflection in the *fa*/Ro relation between 0.7% and 1.0% Ro rather than a single abrupt inflection at 0.7% Ro.

It is to be expected that changes in the development of the chemical structure of vitrinite will be reflected in both changing depth/reflectance relations and changing kinetics, and the limitation of the second stage to 0.7% to 1.0% Ro is similar to the limitation of the inflection in the depth/reflectance relation to 0.7% to 1.0% Ro. Further, it is to be expected that the depth/reflectance gradients would be different before and after the inflection as the changed character of the vitrinites responds differently to increasing temperature. The critical range for the inflection is that of the "oil window".

CONCLUSIONS

(1) Vitrinite reflectance is a useful but imprecise indicator of the degree of diagenetic and metamorphic progress in sediments. In particular, the trends within a sequence are more important than individual determinations.
(2) Based on the depth/reflectance relations in >25 wells with useful ranges of reflectance values, reflectance initially increases linearly to 0.7% Ro, then rapidly to 1.0% Ro, and then again linearly but at a greater rate than it did initially.
(3) Depth/reflectance relations should be illustrated using linear scales for both parameters, rather than the commonly-used linear scale for depth and log scale for reflectance. The marked inflection between 0.7% and 1.0% Ro tends to be obscured if a semi-log diagram is used, to the extent that some authors have supposed that the characteristic depth/reflectance relation is a straight line on that diagram.
(4) The depth/reflectance relations depend systematically on the geothermal gradients at the time that the reflectance values were set, usually at the time of maximum depth of burial in a sedimentary basin. Accordingly, a general diagram relating depth, reflectance and geothermal gradient can be constructed (Fig. 5).
(5) Using this general diagram, estimates of former maximum depths of burial and paleogeothermal gradients can be made from the depth/reflectance relations in wells that now have incomplete sections as a result of erosion at the present-day surface or the development of an unconformity within the subsurface sequence.
(6) The inflection between 0.7% and 1.0% Ro, and the estimates of both maximum depths of burial and paleogeothermal gradients, need to be considered, together with other inputs including changing kinetics, when developing and testing models of thermal histories of wells.
(7) The inflection between 0.7% and 1.0% Ro is related to the changing chemistry of vitrinite during oil generation. The different linear gradients above and below this inflection are correspondingly related to the differences in reactions associated with the chemistry of pre-mature and post-mature vitrinite.

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