Comparison of Maturation Data and Fluid-inclusion Homogenization Temperatures to Simple Thermal Models: Implications for Thermal History and Fluid Flow in the Midcontinent

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Abstract

Time-temperature index (TTI) modeling is used to establish a simple theoretical thermal maturity for Paleozoic strata in central Kansas. These thermal maturation calculations are based on estimates of likely geothermal gradients and best knowledge of the tectonic history of the region, as derived from stratigraphic thicknesses and estimates of erosion at unconformities. Major uncertainties in the data for the TTI modeling are burial during Cretaceous time and geothermal gradient, thus several models were calculated in which ranges of these two variables were considered. Results of the thermal modeling are then compared to available data on the thermal maturation. These data are principally derived from subsurface samples, on which vitrinite-reflectance, pyrolysis, and fluid-inclusion analyses have been performed.

Vitrinite-reflectance and Rock-Eval maturation measurements indicate that Middle and Upper Ordovician strata (i.e., Simpson, Viola, and Maquoketa formations) in the study area are in initial phases of oil generation. Maturation modeling can match the results of the organic analyses, but geothermal gradients and burial during the Cretaceous have to be maximized.

Although the TTI modeling utilizing very high geothermal gradients and near-excessive thicknesses of Cretaceous strata can match the observed maturation, the modeled results are probably not correct because fluid-inclusion data from saddle dolomites from the Upper Ordovician Viola Limestone indicate this unit reached temperatures 50°C higher than the maximum modeled temperature. A thermal event is inferred to account for the excess maturation and elevated fluid-inclusion homogenization temperatures. This thermal event may be manifested in the erratic increase of vitrinite-reflectance with depth for post-Devonian strata, as well as for pyrolysis measurements in wells for which maturation profiles are available. Flow of heated water onto the cratonic shelf out of the Anadarko basin during the late Paleozoic Ouachita orogeny may be responsible for the maturation anomalies.

Past thermal regimes and regional fluid flows have recently been considered as processes affecting the distribution of petroleum, minerals, and diagenesis in the midcontinent. Studies in the last 10 years (Gregg, 1985; Leach and Rowan, 1986; Bethke and Marshak, 1990; Barker et al., 1992; Ge and Garven, 1992; Wojcik et al., 1992, 1994; Luczaj, 1995; Walton et al., 1995) have invoked general northward flow of heated fluids onto the cratonic shelf out of the deep Anadarko and Arkoma basins. High-temperature basinal fluids have been postulated to account for lateral changes in chemistry and mineralogy of lead-zinc districts in southern Missouri, Kansas, and Arkansas (Gregg, 1985; Leach and Rowan, 1986), and for the contiguous occurrence of petroleum from the deep Anadarko basin of Oklahoma to the relatively thin strata of central Kansas (Rich, 1933; Walters, 1958; Price, 1980).

Inference of an ancient thermal regime that was hotter than the current one principally relies on maturation measurements, such as vitrinite reflectivity or fluid-inclusion homogenization temperatures, that are greater than what can be accounted for by current thermal conditions. If greater-than-expected maturation is measured, then the next step is to determine if this relatively high maturation occurred during a hitherto unexpected period of deep burial or a period of time in which the stratigraphic column was temporarily affected by greater heat flow. If excessive heat flow is indicated, it is important to determine whether this heat was principally transferred by conduction or by a flux of heated fluid from elsewhere.

The inadequacy of simple thermal models to fit available maturation and temperature data is either explained by thermal perturbation or poor assumptions of

TABLE 1. Correlation of time-temperature index (TTI), Rock-Eval transformation ratio (TR), and Rock-Eval T_{max} to vitrinite reflectance (R_o). TTI to R_o is from Waples, 1981; TR and T_{max} to R_o is from Peters, 1986.

Stage	TTI	TR	T_{max} (°C)	R_o (%)
Onset of oil generation (Peters)		~0.1	~435-445	~0.6
Onset of oil generation (Waples)	15			0.6
Peak oil generation (Waples)	75			1.1
End oil generation (Waples)	160			1.3
End oil generation (Peters)		~0.4	~470	~1.4
Upper TTI limit for wet gas (Waples)	1,500			~3.8

the simple thermal model. If the assumption of simple burial heating can be shown to have been unlikely, then additional heating events, possibly ephemeral or short-lived, may have to be invoked. Understanding the thermal history is important, for it is intimately linked with the geologic evolution of the setting, its petroleum occurrence, and mineralization. In particular, orogenic belts, with their adjacent forelands and cratonic basins, have linked geologic histories. If significant transfer of heat from an orogenic belt into an adjacent shallow cratonic basin can occur by processes such as fluid movement, then thermal and geologic models that require significant burial and subsequent exhumation of this basin may be in error. Inasmuch as petroleum-exploration strategies and models of resource emplacement largely depend on concepts of heat transfer and burial history, it is important to evaluate various maturation and temperature data to determine which of the models or geologic processes are correct.

In this paper, organic maturation measurements in Paleozoic strata and fluid-inclusion temperatures in the Middle and Upper Ordovician rocks in central Kansas will be compared to theoretical maturation calculations produced by a simple model of thermal maturation. This model, a time-temperature index (TTI) calculation, utilizes a geothermal gradient at a given locality and mathematically combines it with a geologic history of subsidence and uplift. It will be demonstrated that the directly measured maturation parameters are higher than can be accounted for by most variations of any geological parameters used to compute the theoretical maturation, and a thermal event is necessary to account for this maturation. Next, spatial and stratigraphic characteristics of the maturation measurements will be examined to determine whether this anomalous maturation is due to fluid flow or a temporary flux of conductive heat from basement rocks. Evidence favors the former process.

TTI Modeling for Localities in Central Kansas

Procedures for TTI Calculation

A time-temperature index model (Waples, 1980; 1981), based on work by Lopatin (1971), takes into account both time and temperature in calculating a cumulative thermal maturity for sedimentary organic matter. This technique assumes that the rates of chemical reactions involved in the conversion of kerogen to petroleum can be mathematically approximated by a first-order chemical reaction in which the rate of maturation doubles for every 10°C rise in temperature. The Lopatin technique generates a dimensionless number, called the "time-temperature index" (TTI) that Waples (1981) empirically correlated to vitrinite reflectivity and stages of oil and gas generation (table 1). The TTI models were run with a geothermal gradient that did not vary over geologic time, but with a surface temperature that changed according to paleoclimate and global position of Kansas over geologic time. The tectonic history was depicted by plotting subsidence and uplift of various strata against time. Subsidence was determined by thicknesses and ages of strata; uplift was determined by estimating erosion that occurred at major unconformities. The graphical history of subsidence and uplift and of subsurface temperatures was also utilized to infer the maximum temperature and depth a given stratigraphic interval experienced and the time at which various levels of maturation were achieved. Refinements can be added to the TTI calculation, such as decompacting the sedimentary column and taking into account heat flow and thermal conductivity of individual rock layers to determine the geothermal gradient. In this study, however, only limited organic and thermal maturation data were available with which to compare the results of such elaborate modeling, so the models presented were kept simple.

TTI calculations are specific only to a single locality—usually one well. In this study, two localities were selected: a location at the crest of the Central Kansas arch in western McPherson County (T. 19 S., R. 4 W.), and a location in southern Harper County (T. 33 S., R. 7 W.) where the Viola Limestone is deepest in central Kansas (fig. 1). The localities were selected to provide answers to the following questions: (1) What is the maximum temperature and depth to which the Upper Ordovician Viola Limestone in central Kansas has been subjected? (2) When did the Viola Limestone experience these conditions? (3) How well do direct maturation indicators compare to the thermal maturity indicated by the TTI modeling? (4) Are additional thermal events necessary to better correlate the TTI modeling to the direct maturation indicators?

Input: Most Likely Range of Geologic Parameters

Although geothermal gradient is important for TTI calculations, it is a hard-to-determine parameter because temperature data, principally derived from oil wells after drilling, generally are not measured with precision. To compensate for this imprecision, several TTI models were calculated with a range of likely geothermal gradients. Cretaceous burial was determined to be a second parameter for which there is poor control, and TTI models were also run with varying thicknesses of Cretaceous strata. Other input parameters for the two localities modeled are discussed below.

Geothermal Gradients. Maps based on bottom-hole temperature (BHT) measured during wireline logging (e.g., Stavnes, 1982; Stavnes and Steeples, 1982; American Association of Petroleum Geologists, 1976) indicate the geothermal gradient in McPherson County (the northern part of the study area) is approximately 25°C/km, but nearby wells that have been thermally logged (Stavnes, 1982) indicate a gradient of approximately 30°C/km (fig. 1). The geothermal gradient in Harper County (the southern part of the study area) is approximately 25°C/km according to BHT data, but nearby wells at thermal equilibrium with surrounding rock have recorded gradients as high as 40°C/km (Stavnes, 1982) (fig. 1). The difference in geothermal gradient is caused by several factors, including inadequate time for thermal equilibration of the well bore with the surrounding rock and differences in thermal conductivity of the strata being logged (Deming et al., 1990; Förster and Merriam, 1993; Förster et al., 1993).

Stratigraphic Data. Average surface temperatures used in the TTI modeling are presented in table 2. Stratigraphic data for McPherson and Harper counties are presented in tables 3 and 4, respectively. Uncertainties in the history of subsidence and uplift stem from the numerous unconformities that are characteristically present on the craton. Phanerozoic time in the midcontinent is dominated by erosion and nondeposition; 50–85% of this time is represented by unconformities (Merriam, 1963). Although

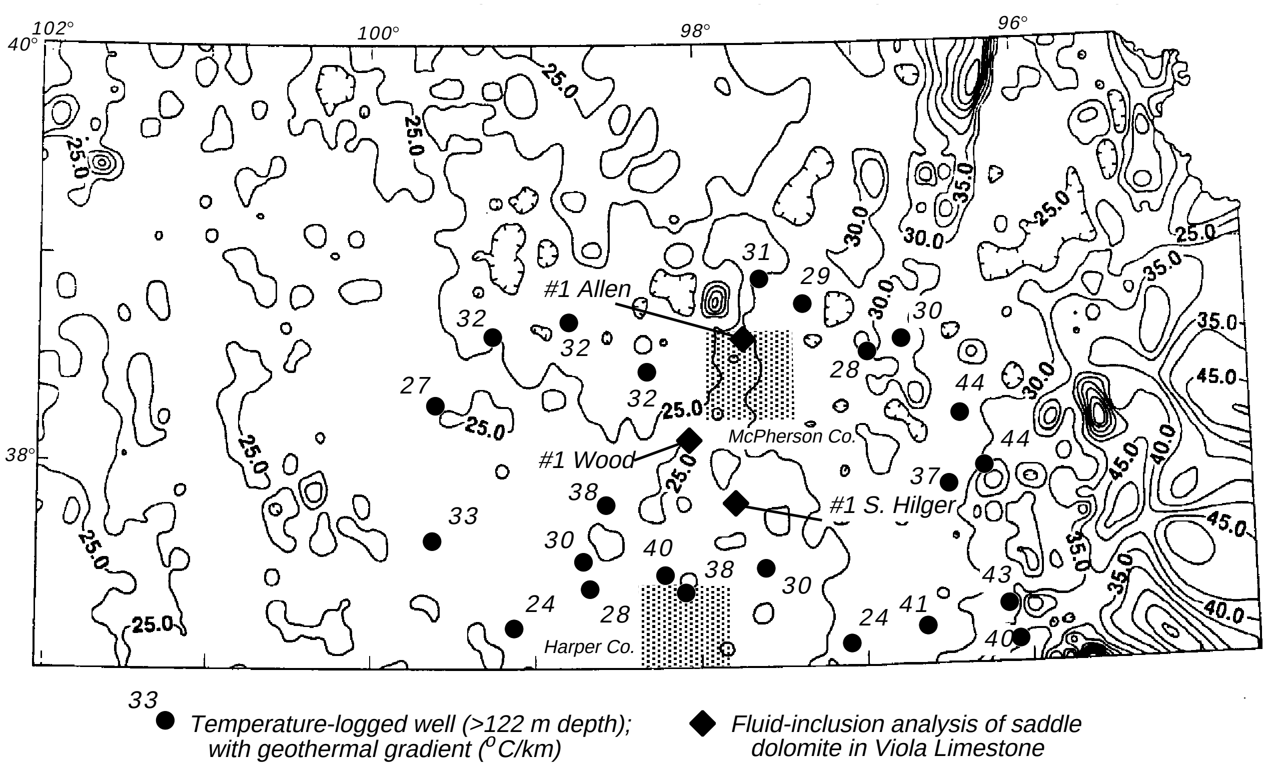


FIGURE 1. A geothermal gradient map of Kansas based on 43,348 bottom-hole temperatures (BHT's) from oil and gas tests (Stavnes and Steeples, 1982). Counties targeted for TTI modeling are shaded; wells in which saddle dolomites were analyzed for fluid-inclusion homogenization temperatures are superimposed on the geothermal gradient map. Temperature-logged wells (Stavnes, 1982) in the vicinity of the modeling localities are also shown, along with their determined geothermal gradients. Isopleths are at 5°C/km. Generally higher geothermal gradients in eastern Kansas are attributable to data derived from many relatively shallow wells that were drilled only into Pennsylvanian strata. Because strata are characterized by relatively low thermal conductivity, temperatures rise relatively rapidly with depth; consequently, a BHT measurement from a shallow well in this locality generally will yield an anomalously higher geothermal gradient (Förster and Merriam, 1993).

TABLE 2. Change of mean surface temperature with time (from Habicht, 1979); surface temperature is assumed to change in a linear fashion between the temperature nodes and times. Times are given in million years before the present (Ma).

Age	Mean Surface Temperature (°C)
Present (0 Ma)	12
Late Tertiary (5 Ma)	14
Early Tertiary (40 Ma)	18
Cretaceous (103 Ma)	20
Jurassic (175 Ma)	24
Triassic (230 Ma)	29
Permian (270 Ma)	30
Carboniferous (325 Ma)	24
Devonian (385 Ma)	26
Silurian (425 Ma)	27
Ordovician (470 Ma)	20
Cambrian (545 Ma)	26

the geologic record is incomplete, lower Paleozoic units (i.e., Arbuckle, Simpson, Viola, Maquoketa, "Hunton," Chattanooga, and Mississippian strata) are characterized by only mild deformation, with relative dips between units varying less than 5 degrees (Lee, 1956). The thinness of these units compared to their lateral extent also suggests that significant subsidence and uplift were not the norm during the early Paleozoic and that the maximum preserved thickness of individual units is probably close to their original compacted thickness, despite unconformities usually present at the tops of these units. Furthermore, because little maturation occurs at such shallow depths, gaps in sedimentation in the lower Paleozoic section are relatively inconsequential for purposes of TTI calculations.

The lower Paleozoic units were buried relatively deeply by the end of Paleozoic time; therefore, the burial history after Paleozoic time is important. Unfortunately, much of this history has been erased by subsequent erosion. Cretaceous rocks are the thickest of the Mesozoic rocks in Kansas (Merriam, 1963), but the original thickness of these strata in central Kansas is difficult to estimate due to erosion. Cretaceous rocks in northwestern Kansas reach 3,000 ft (920 m) in thickness but are completely eroded in the eastern part of the state (Merriam, 1963). Graphical projection of Cretaceous thicknesses to the McPherson County locality from regional cross sections (Merriam, 1963) indicate Cretaceous strata deposited there were at least 1,500 ft (460 m) but probably did not exceed 3,000 ft (920 m). The thickness of Cretaceous strata deposited in Harper County was presumably less than in McPherson County because this area was on the flank of the Ozark dome, which was a geographical feature during Mesozoic time (Merriam, 1963). The thickness of Cretaceous strata at the Harper County locality is estimated to be 500 ft (150 m). Erosion of Cretaceous strata presumably began at the beginning of the Laramide orogeny in Late Cretaceous to Early Tertiary time, and this erosion is assumed to have been continuous up to the present. Strata deposited during the Cenozoic in Kansas is relatively thin and thus inconsequential for purposes of TTI modeling.

TABLE 3. Subsidence and uplift of basement in McPherson County. Duration of tectonic movement is given in Ma (absolute ages derived from Haq and Van Eysinga, 1987); formation names or age subdivisions, for reference, are in parentheses.

Age (and unit)	Ma	Subsidence	Uplift
Cambrian–Ordovician (Arbuckle)	524–478	550 ft (168 m)	—
	478–466	—	50 ft (15 m)
Ordovician (Simpson, Viola)	466–446	200 ft (61 m)	—
Ordovician (Maquoketa)	446–440	50 ft (15 m)	—
Silurian ("Hunton")	440–422	250 ft (76 m)	—
	422–388	—	—
Devonian ("Hunton")	388–376	50 ft (15 m)	—
	376–368	—	300 ft (91 m)
Devonian–Mississippian (Chattanooga)	368–340	350 ft (107 m)	—
Mississippian strata	340–326	325 ft (99 m)	—
	326–310	—	100 ft (30 m)
Pennsylvanian strata (Desmoinesian)	310–306	300 ft (91 m)	—
Pennsylvanian strata (Missourian)	306–302	325 ft (99 m)	—
Pennsylvanian strata (Virgilian)	302–290	1,000 ft (305 m)	—
Permian strata	290–250	2,250 ft (686 m)	—
	250–140	—	550 ft (168 m)
Cretaceous strata[1]	140–68	1,500 ft (457 m)[1]	—
	68–0	—	1,950 ft (594 m)

[1]Cretaceous thickness variable, but all of Cretaceous strata, plus 450 ft (137 m) of underlying Permian strata, was modeled as eroded from 68–0 Ma.

TABLE 4. Subsidence and uplift of basement in Harper County. Duration of tectonic movement is given in Ma (absolute ages derived from Haq and Van Eysinga, 1987); formation names or age subdivisions, for reference, are in parentheses.

Age (and unit)	Ma	Subsidence	Uplift
Cambrian–Ordovician (Arbuckle)	524–478	1,050 ft (320 m)	—
	478–466	—	50 ft (15 m)
Ordovician (Simpson, Viola)	466–446	150 ft (46 m)	—
Ordovician (Maquoketa)	446–440	—	—
Silurian (“Hunton”)	440–422	—	—
	422–388	—	—
Devonian (“Hunton”)	388–376	—	—
	376–368	—	50 ft (15 m)
Devonian–Mississippian (Chattanooga)	368–340	125 ft (38 m)	—
Mississippian strata	340–326	325 ft (99 m)	—
	326–324	—	100 ft (30 m)
Pennsylvanian strata (Morrowan–Atokan)	324–310	325 ft (99 m)	—
Pennsylvanian strata (Desmoinesian–Virgilian)	310–290	1,775 ft (541 m)	—
Permian strata	290–250	2,875 ft (876 m)	—
	250–140	—	175 ft (53 m)
Cretaceous strata	140–68	500 ft (152 m)	—
	68–0	—	600 ft (183 m)

Output: Results of Calculations

A tectonic mobility diagram and temperature history for McPherson County (fig. 2) shows the Viola Limestone reaching a maximum burial temperature of 70°C at the end of the Permian. This particular model illustrates a 30°C/km constant geothermal gradient and 1,500 ft (460 m) of Cretaceous strata. With this model, the beginning of significant oil generation (TTI = 15) would have started in the Simpson Group (directly beneath the Viola Limestone), in Late Cenozoic time (fig. 2). The Viola Limestone, like the Simpson Group, would therefore be marginally mature with respect to oil generation. A high-end estimate of 3,000 ft (920 m) of Cretaceous strata, in conjunction with a 30°C/km would have subjected the Viola Limestone to a maximum burial temperature of 85°C at the end of the Cretaceous; a 40°C/km gradient would produce a maximum burial temperature of 105°C at the end of the Cretaceous.

The results of several TTI models for McPherson County with different geothermal gradients and Cretaceous cover are expressed in two nomograms that show the TTI calculated for the top of the Simpson Group, the base of Viola Limestone (fig. 3), and the base of the Pennsylvanian section (fig. 4). Most combinations of likely geothermal gradients and Cretaceous thicknesses at this location will put the Simpson Group into the oil window, but below the peak of oil generation (i.e., $15 < TTI < 75$), whereas the Pennsylvanian section would be in the initial stages of oil generation (fig. 4).

Because less Cretaceous cover is expected at the Harper County location, the calculated maturation in that area is principally dependent on geothermal gradient. The extremes in the geothermal gradient, as estimated with BHT’s and the temperature-logged wells are 25°C/km and 40°C/km, respectively (fig. 1). With a geothermal gradient of 25°C/km, the Viola Limestone would experience a maximum temperature of 70°C at the end of the Permian (fig. 5). With a geothermal gradient of 40°C/km, the Viola Limestone would reach a maximum temperature of 95°C at the end of the Permian (fig. 5).

Direct Maturation Indicators

Most lower Paleozoic shelf limestones in Kansas, including the Viola Limestone, have a low organic content, hence the relatively organic-rich units that stratigraphically bracket the Viola Limestone (e.g., dark shales from the Middle Ordovician Simpson Group, the Upper Ordovician Maquoketa Shale, and the Devonian-Mississippian Chattanooga Shale) are used to interpolate its maturation. The most common analyses of thermal maturation using organic materials involve Rock-Eval pyrolysis and vitrinite reflectance. These analyses have been compiled for several wells in central Kansas and aid in evaluating the results of the TTI modeling.

Another source of data is homogenization temperatures (T_h) of fluid inclusions in saddle (baroque) dolomites. Saddle dolomite is present in the Viola Limestone as a late-stage diagenetic phase filling vugs and molds. T_h measurements were performed using a Fluid, Inc. adapted U.S.G.S. gas-flow heating/freezing stage attached to an optical microscope. Doubly polished thin sections used for the fluid-inclusion microscopy were made using cold techniques, in order to avoid thermal damage to the fluid inclusions.

Rock-Eval Data: Transformation Ratio and T_{max}

Maturation of lower Paleozoic strata can be semi-quantitatively evaluated using Rock-Eval pyrolysis. Four

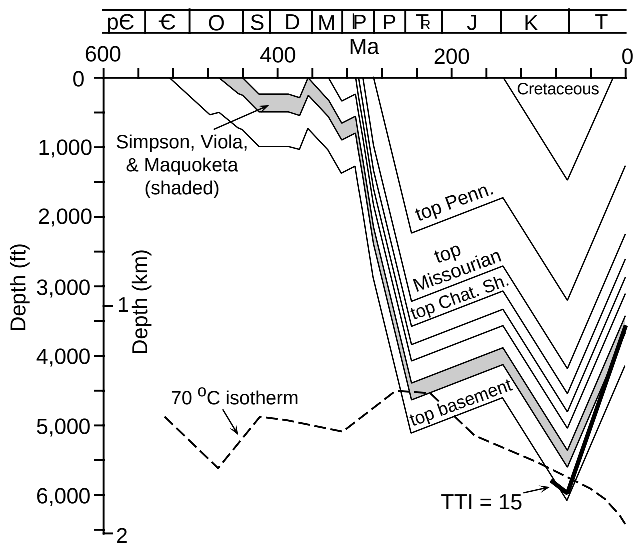


FIGURE 2. A tectonic mobility diagram and temperature history for the area in McPherson County. This particular model illustrates a 30°C/km constant geothermal gradient and 1,500 ft (460 m) of Cretaceous strata. The Viola Limestone would attain a maximum burial temperature of 70°C at the end of the Permian according to this thermal and subsidence history. The start of significant oil generation, represented by TTI = 15, is shown rising through the stratigraphic section with time, reaching the base of the Simpson Group at about the mid-Tertiary.

basic parameters (S_1, S_2, S_3, and T_{max}) are obtained by this method (Espitalié et al., 1977). S_1 (expressed as mg HC/g rock, or the equivalent measure of kg HC/metric ton rock) measures free or adsorbed hydrocarbons present in the rock. S_2 (expressed as mg HC/g rock, or kg HC/metric ton rock) measures pyrolitic hydrocarbons derived from thermal breakdown of kerogen. The temperature at which maximum pyrolitic hydrocarbon yield occurs is T_{max}. S_3 (expressed as mg CO_2/g rock, or kg CO_2/metric ton rock) measures pyrolitic carbon dioxide yielded by the sample.

Ratios of these parameters can be used as approximate measures of maturation (Espitalié et al., 1977). $S_1/(S_1 + S_2)$ defines the transformation ratio (TR). TR increases with thermal maturation until expulsion of hydrocarbons take place. According to Tissot and Welte (1984) and Peters (1986), the oil window corresponds to a TR range between 0.1–0.4 (table 1). T_{max} also increases with thermal maturation. The oil window according to T_{max} lies between 435°C and 470°C, with the caveat that T_{max} values signaling the beginning of significant oil generation may vary according to the type of organic matter (Peters, 1986) (table 1). T_{max} values for type I organic matter, which typifies some pre-Devonian rocks, commonly has a narrow range of variation between 435°C and 450°C (Tissot et al., 1987).

Figures 6 and 7 show the T_{max} and TR data collected for north-central Kansas, which apply to the area modeled in McPherson County. No data are available close to the locality modeled in Harper County. In spite of scatter, these results indicate that Ordovician strata in Kansas are immature or are in early stages of oil generation. Slightly higher maturity generally is registered by the TR data, but onset of oil generation is still indicated. The measured level of maturation can be accommodated by the results obtained by the TTI modeling. As higher geothermal gradients are assumed, lesser thicknesses of Cretaceous rocks have to be assumed in order to obtain a similar level of maturity. The model suggests that geothermal gradients greater than 25 to 30°C/km are not indicated because amount of Cretaceous strata would have to be unrealistically thin at the McPherson County locality (fig. 3).

The wells in the vicinity of McPherson County show a slight increase in T_{max} and TR with depth (fig. 8). Variations in levels of maturation are evident between wells,

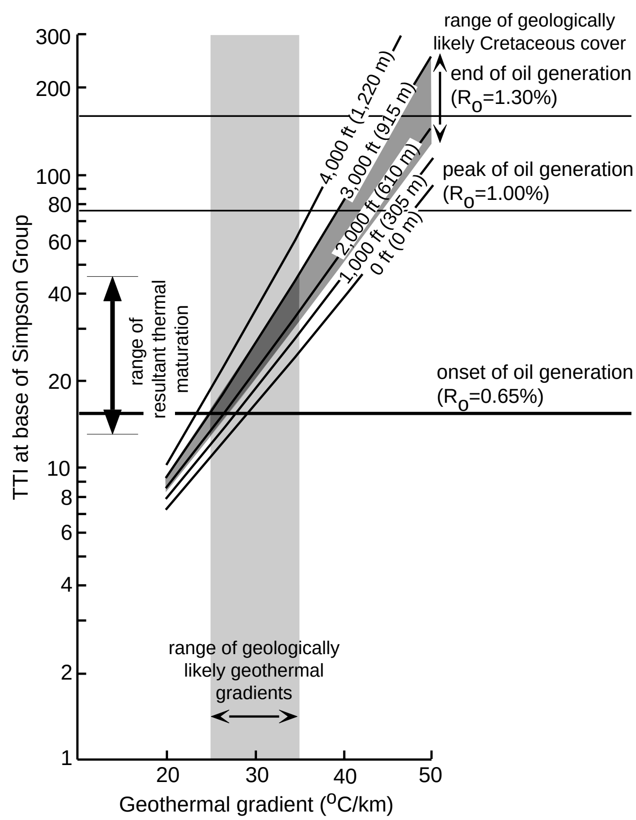


FIGURE 3. A nomogram expressing the results of TTI modeling at McPherson County as a consequence of geothermal gradient and depth of Cretaceous burial for the top of the Simpson Group (i.e., base of Viola Limestone). To read the TTI, extend a geothermal gradient from the base of the diagram in a vertical line to the assumed thickness of Cretaceous rocks (shown by diagonal lines). The resultant TTI is determined by extending a horizontal line left from the point at which the lines depicting the geothermal gradient and Cretaceous cover intersect. The ranges of geologically likely geothermal gradients and Cretaceous cover are shaded in yellow and blue, respectively. Most likely combinations of these (where the yellow and blue overlap) puts the Simpson Group and Viola Limestone into initial stages of oil generation.

and with depth for each well. Even though the effects of depth and stratigraphy are largely removed by plotting the maturation profiles relative to the basal Pennsylvanian unconformity (Wojcik et al., 1994), differences in maturation between wells are still evident. Inasmuch as these wells largely have similar stratigraphy at the basal Pennsylvanian unconformity (i.e., nearly identical units are present both below and above this unconformity), the consistent difference in maturity at given stratigraphic levels is most likely due to a variation in thermal history experienced at each locality. For example, the T_{max} values at the Diamond-Shamrock #1-9 Skully well indicate consistently greater maturation than those recorded at the nearby Walker #1 Unruh well. Thermal conductivities at both wells are similar due to their nearly identical stratigraphy; therefore, a locally higher heat flow or localized advective heat transport would be the most likely explanation for the greater maturation at the Diamond-Shamrock #1-9 Skully well.

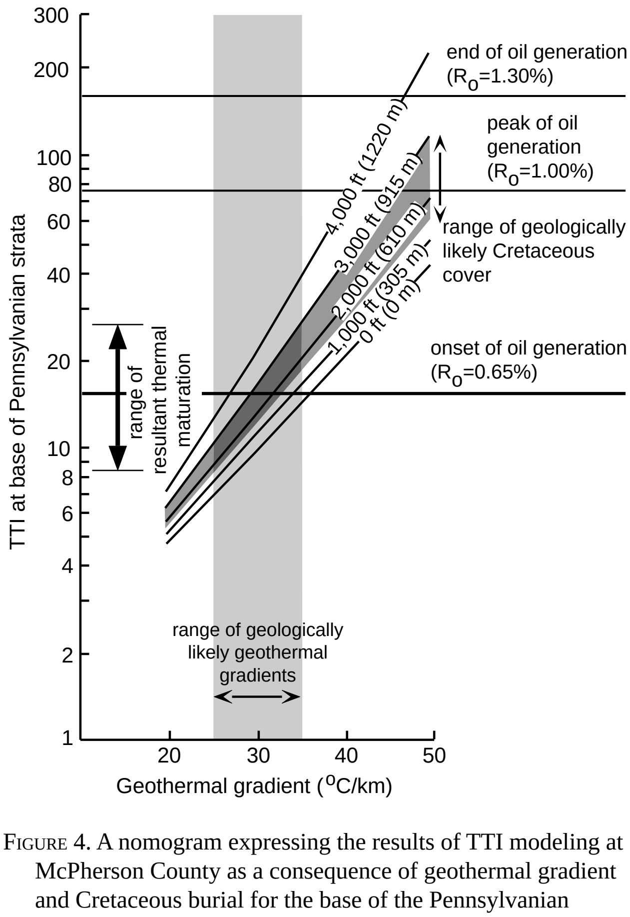


FIGURE 4. A nomogram expressing the results of TTI modeling at McPherson County as a consequence of geothermal gradient and Cretaceous burial for the base of the Pennsylvanian section. See fig. 3 for instructions for obtaining TTI. Most likely combinations of geothermal gradients and Cretaceous cover indicate the base of the Pennsylvanian section would be immature to only marginally mature with respect to oil generation.

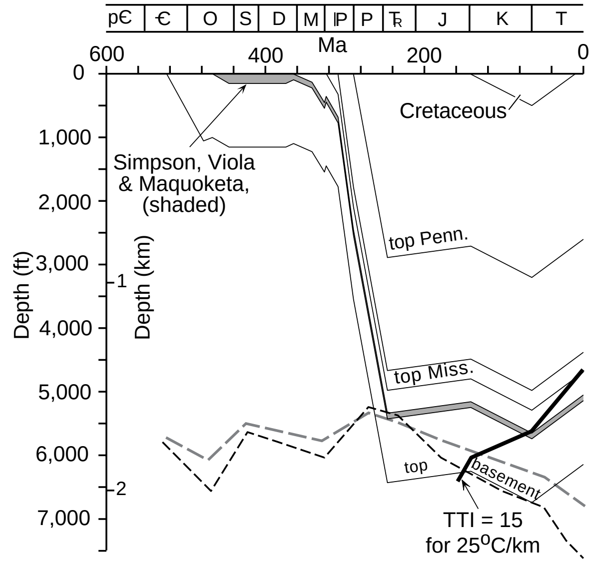


FIGURE 5. A tectonic mobility diagram and temperature history for the area in Harper County. This particular model illustrates maturation associated with a 25°C/km constant geothermal gradient. The Viola Limestone would attain a maximum burial temperature of 70°C at the end of the Permian according to this thermal and subsidence history, as shown in the superimposed isotherm (heavy dashed line). Also superimposed on this diagram is a 90°C isotherm (light dashed line), which is the maximum burial temperature the Viola Limestone would experience if a 40°C/km constant geothermal gradient were assumed. The start of significant oil generation, represented by TTI = 15, is shown rising through the stratigraphic section with time, reaching the base of the Simpson Group at about the end of the Cretaceous.

Vitrinite-Reflectance Data

Vitrinite is an organic maceral derived from the tissue of terrestrial plants (Tissot and Welte, 1984). With increasing thermal maturity, vitrinite undergoes progressive, irreversible graphitization and consequently its reflectivity increases. Direct assessment of the thermal maturity of lower Paleozoic rocks by vitrinite reflectance is not feasible because terrestrial plants are not present in pre-Silurian rocks (Hunt, 1979). Vitrinite reflectance (R_o) is the most commonly used quantitative thermal maturation indicator in the oil industry and several scales correlating it to stages of oil generation have been established (cf., Héroux et al., 1979; Waples, 1980; Dow and O'Connor, 1982; van Gijzel, 1982; Tissot and Welte, 1984). In general, R_o values from 0.5 to 1.4% (±0.1%) correspond to the range of maturation in which oil is generated, with the peak of oil generation occurring about 1.0% R_o (fig. 9; also see table 1).

The correlation of TTI to R_o values by Waples (1980, 1981) (table 1) has been amended by recent publications. For example, by a linear relationship between R_o values and TTI, Morrow and Issler (1993) equated 0.7% R_o to a TTI of 50; Waples (1980) equated it to a TTI of 10 to 20.

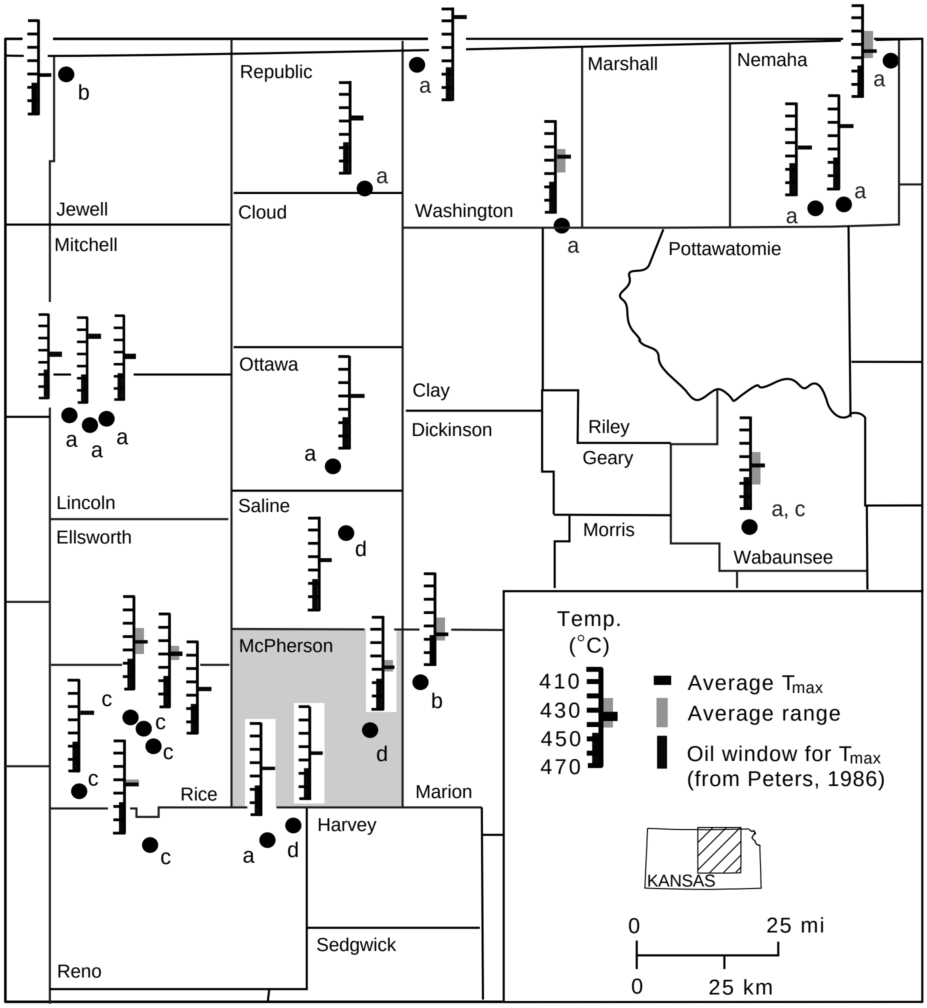


FIGURE 6. Thermal maturation of Middle and Upper Ordovician strata in north-central Kansas as expressed by Rock-Eval T_{max} data. These data indicate Middle and Upper Ordovician strata in Kansas are immature to marginally mature with respect to petroleum generation. A listing of these samples is in Appendix II in Newell (1996). Letter by each well location denotes the source of the analyses: a = DGSI (1986–1994), b = Sohio (Irene Penfield, personal communication, 1984–1985), c = U.S. Geological Survey (Joseph Hatch, personal communication, 1984–1985), d = Brown & Ruth (Susan Landon, personal communication, 1984). Samples analyzed by DGSI were tested by procedures outlined in Jarvie (1991) for ascertaining total organic carbon (TOC). Pyrolysis data on these samples were obtained using a Rock-Eval II instrument (Philp and Galvez-Sinibaldi, 1991). Kerogen inspected by microscopy were prepared by techniques in Dow and O'Connor (1982). Instrumentation used by remaining sources is unknown. Core samples and cuttings for all analyses were hand-picked and washed with distilled water to remove impurities. Rock-Eval pyrolysis was performed on samples with TOC > 0.2 wt. %.

According to these more recent findings, the models presented in this report would have to assume even higher geothermal gradients, deeper burials, or both, to account for the R_o measurements taken near the modeling localities. Numerical models of maturation, as well as the correlation of the calculations to directly observed maturation parameters, are beyond the scope of this paper. However, it is significant that even with the tendency of the Waples correlation to perhaps overestimate maturation in terms of vitrinite-reflectance equivalency, the calculated maturation generally is still less than the observed maturation.

McPherson County. Published and new R_o maturation data for Kansas show Pennsylvanian shales in the vicinity of McPherson County with R_o values of 0.5–0.7% (fig. 9). Maturation around Harper County is slightly greater, with R_o ranging from 0.6–0.8% in the Pennsylvanian section. According to TTI-to-R_o correlations from Waples (1980) (table 1), an R_o between 0.6–0.7% corresponds to a TTI from 10 to 20. If the high end of the R_o range is accepted for the base of the Pennsylvanian System for the locality modeled at McPherson County (i.e., 0.7% R_o, which corresponds to TTI = 20), and the thickness of Cretaceous rocks is kept at 1,500 ft (460 m), a geothermal gradient of

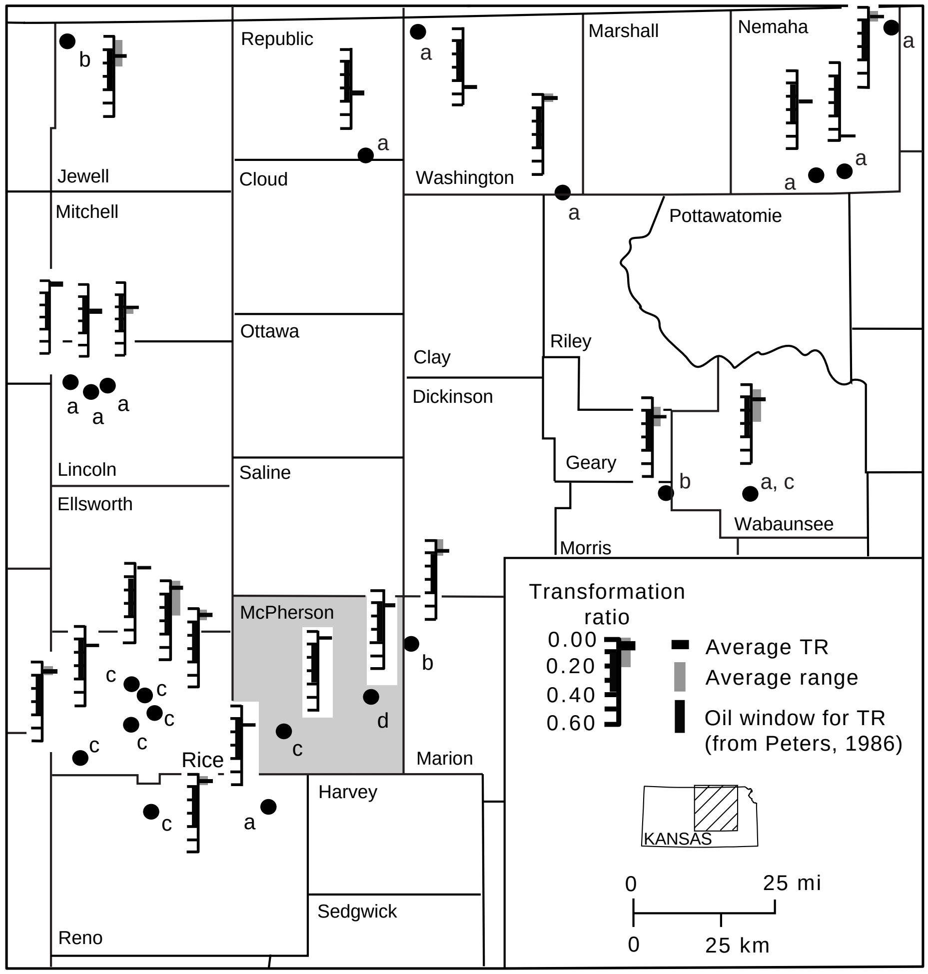


FIGURE 7. Thermal maturation of Middle and Upper Ordovician strata in north-central Kansas as expressed by Rock-Eval transformation ratios (TR). A listing of these samples are in Appendix II in Newell (1996). Although slightly higher maturities are indicated by the TR data than with the T_{max} data (fig. 6), immature to marginal maturity with respect to petroleum generation is still indicated. Letter by each well location denotes the source of the analyses: a = DGSI (1986–1994), b = Sohio (Irene Penfield, personal communication, 1984–1985), c = U.S. Geological Survey (Joseph Hatch, personal communication, 1984–1985), d = Brown & Ruth (Susan Landon, personal communication, 1984). Samples analyzed by DGSI were tested by procedures outlined in Jarvie (1991) for ascertaining total organic carbon (TOC). Pyrolysis data on these samples were obtained using a Rock-Eval II instrument (Philp and Galvez-Sinibaldi, 1991). Kerogen inspected by microscopy were prepared by techniques in Dow and O'Connor (1982). Instrumentation used by remaining sources is unknown.

approximately 40°C/km would be necessary to account for this maturation (fig. 4). However, this geothermal gradient is higher than the highest values for this area, which range between 25 and 35°C/km, based on local measurements (see figs. 1, 4), and therefore it may be necessary to invoke greater Cretaceous burial instead of increasing the geothermal gradient. The maximum likely Cretaceous thickness of 3,000 ft (915 m) would reduce the necessary geothermal gradient to 32°C/km, which is within the acceptable range of geothermal gradients as constrained by organic maturation in the Simpson Group (figs. 3, 4). A geothermal gradient of 32°C/km in conjunction with 3,000 ft (915 m) of Cretaceous burial would subject the Viola Limestone to a maximum burial temperature of 90°C at the end of Cretaceous time. Inasmuch as Cretaceous cover has to be maximized in the TTI model to account for observed maturation, there is a suggestion that the model, which assumes simple burial heating and constant heat flow, may be inadequate.

Harper County. The greatest vitrinite reflectance (0.8% R_o) for Pennsylvanian strata nearest the locality modeled in Harper County corresponds to TTI = 25 (table 1). A geothermal gradient of 30°C/km at this locality will produce a calculated maturation of TTI = 25 at the base of the Pennsylvanian section; therefore, the lower part of the range of geothermal gradients observed in this region (i.e., 25–40°C/km; see fig. 1) can account for the observed maturation. A model assuming a geothermal gradient of

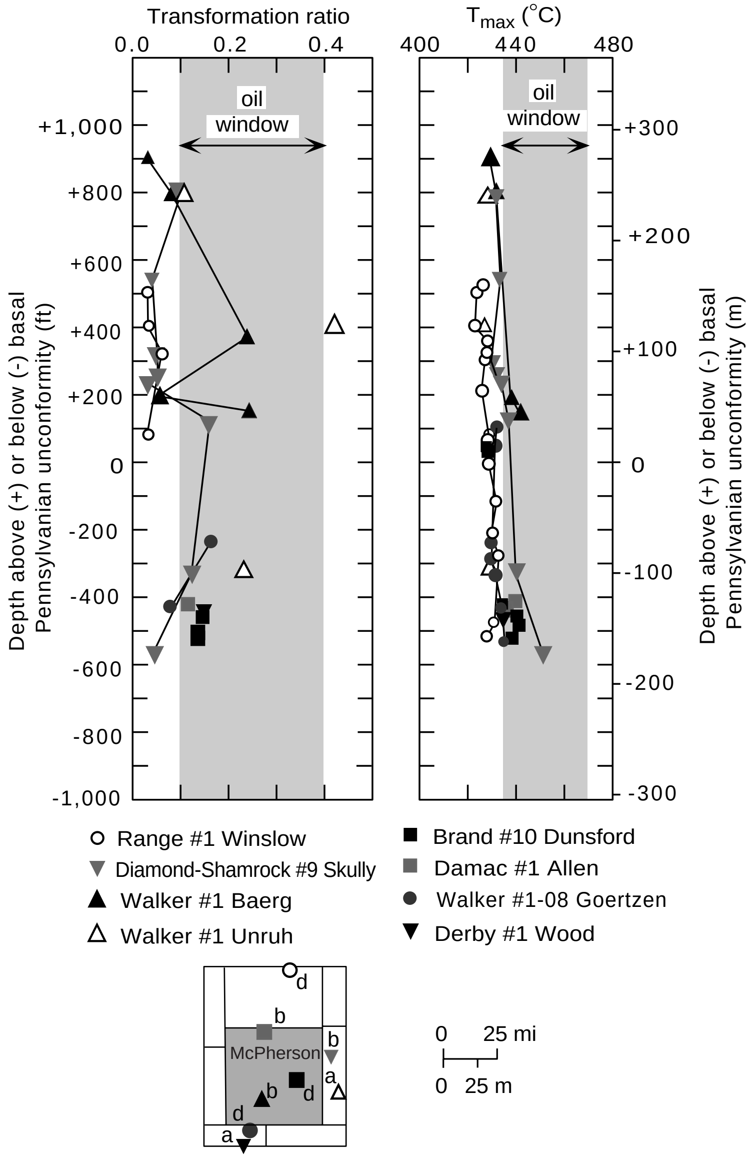
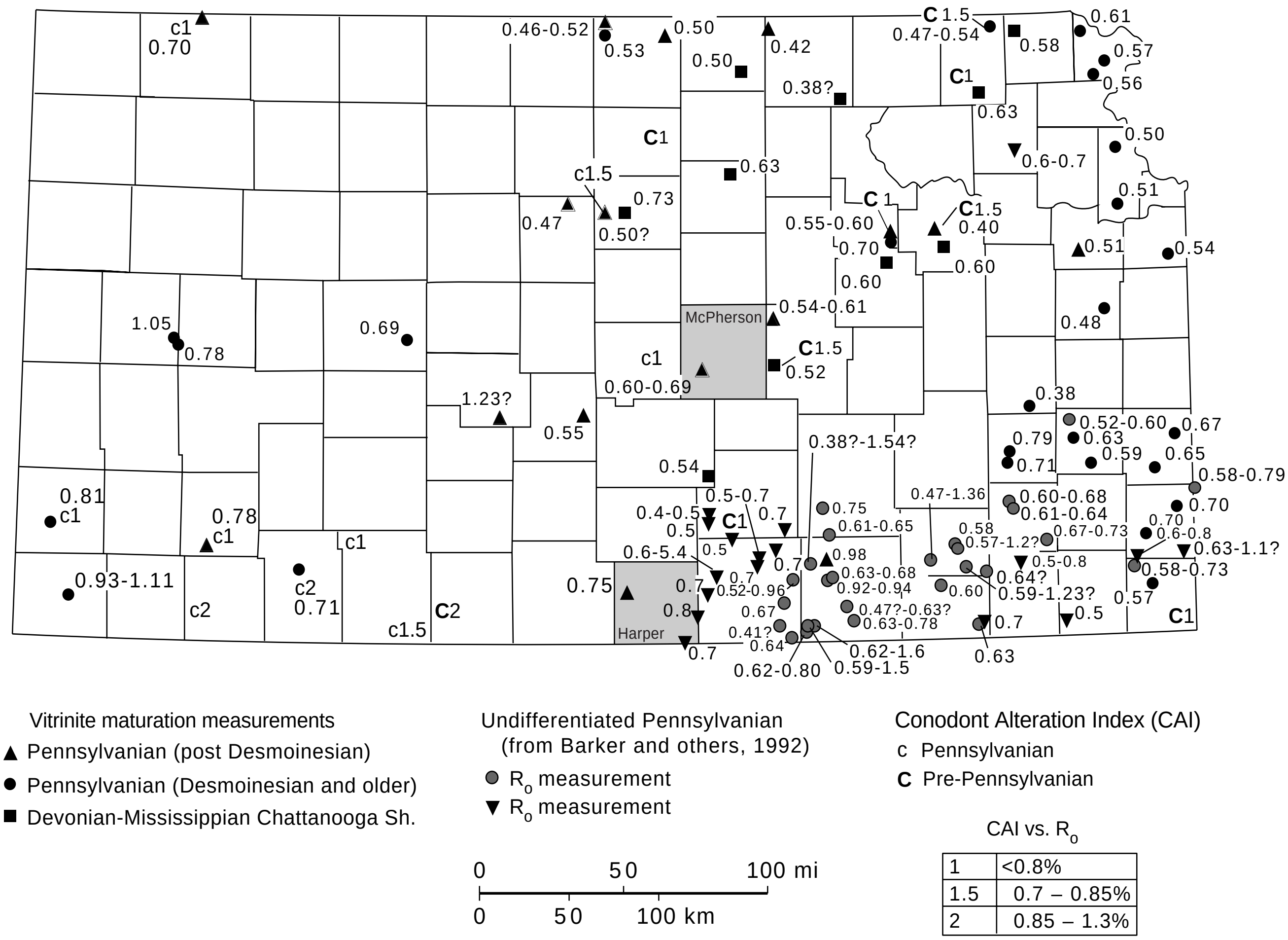


FIGURE 8. Rock-Eval maturation profiles based on T_{max} and TR data for wells in the vicinity of McPherson County, Kansas, plotted by depth in relation to the basal Pennsylvanian unconformity. Lines connect analyses from selected wells. Some of the anomalously high TR values could be due the presence of migrated hydrocarbons, which would inordinately augment the S_1 peak during pyrolysis (Clementz, 1979; Peters, 1986). Compositional variations in the kerogen and rock matrix also may be factors (Tissot et al., 1987). See text for discussion. Letter by each well location denotes the source of the analyses: a = DGSI (1986–1994), b = Sohio (Irene Penfield, personal communication, 1984–1985), c = U.S. Geological Survey (Joseph Hatch, personal communication, 1984–1985), d = Brown & Ruth (Susan Landon, personal communication, 1984). Samples analyzed by DGSI were tested by procedures outlined in Jarvie (1991) for ascertaining total organic carbon (TOC). Pyrolysis data on these samples were obtained using a Rock-Eval II instrument (Philp and Galvez-Sinibaldi, 1991). Kerogen inspected by microscopy were prepared by tech-

30°C/km predicts that the maximum burial temperature experienced by the Viola Limestone in Harper County was approximately 80°C in Permian time.

Vitrinite-reflectance depth profiles (fig. 10), like the Rock-Eval depth profiles in fig. 8, contain scatter and show zones of apparently higher maturation sandwiched between strata with lower maturation. Different maturation at the same stratigraphic horizon between nearby wells (where similar types of organic matter and rock matrix would be expected), and at nearly similar depths (i.e., no great differences in burial history), indicates that the modeling assumptions of simple burial heating and constant heat flow may not be applicable to these rocks. These anomalous zones could be due to compositional variations in organic macerals (Price and Barker, 1985; Tissot et al., 1987) and rock matrix (Law and Nuccio, 1986), or they may even be due to nongeologic causes (Feazel and Aram, 1990). In any case, localized heating,



niques in Dow and O'Connor (1982). Instrumentation used by remaining sources is unknown.

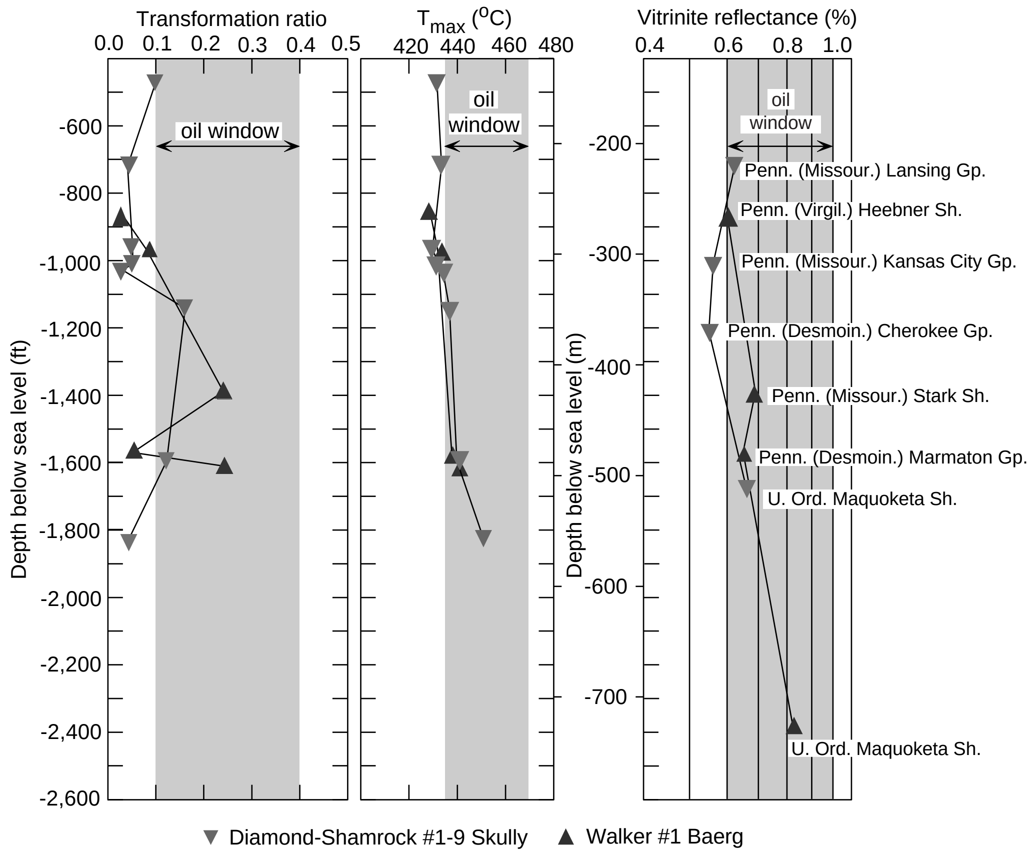
FIGURE 9. Thermal maturation in Kansas as expressed by available published (Jenden et al., 1988; Barker et al., 1992) and unpublished maturation data (Appendices II and III in Newell, 1996). Conodont alteration index (CAI) is a coloration scale applied to the progressive darkening of conodonts with thermal maturation, and can be related to vitrinite reflectance by the conversion in the legend (from Harris, 1979). VRE (vitrinite-reflectance equivalent) data are from Barker et al. (1992), and is based on correlation of T_{max} data with vitrinite-reflectance data from Pennsylvanian rocks in the Cherokee basin. McPherson and Harper counties are

possibly by lateral movement of warm fluids along thin stratigraphic intervals, should not be excluded.

Fluid-inclusion Homogenization Temperatures of Saddle Dolomites

Homogenization temperatures (T_h) measurements can be compared to the maximum burial temperature modeled for the Viola Limestone. To do this, T_h from saddle dolomites from three cores taken from the Viola Limestone (e.g., Damac #1 Sandra Allen in northern McPherson County, Derby #1 Wood in northern Reno County, and Midcontinent Marine #1 South Hilger in southern Reno County) was measured (fig. 1).

The saddle dolomites analyzed are present in vugs and molds and contain abundant fluid inclusions that are varyingly concentrated in zones parallel to crystal faces. Zones such as these are characteristics of growth bands of primary fluid inclusions (Goldstein and Reynolds, 1994). All inclusions observed are two-phase, with consistent liquid-to-vapor ratios, despite differences in sizes of the inclusions. For purposes of fluid-inclusion microscopy, fluid-inclusion assemblages were defined (Goldstein and Reynolds, 1994). In this study, fluid-inclusion assemblages are defined as a group of closely associated inclusions along a growth band. For all three samples, T_h values overlap; the range of all measurements spans about 40°C, with maximum values of 135–140°C (fig. 11). According to Goldstein and Reynolds (1994), in an assemblage derived from a single thermal event, approximately 90% of the fluid inclusions should fall within a temperature interval of 10–15°C. Most fluid-inclusion assemblages in the samples studied have T_h values within a 10–15°C temperature interval. A minimum estimate of the temperature experienced can be inferred as being the highest T_h from a consistent fluid-inclusion assemblage (Goldstein



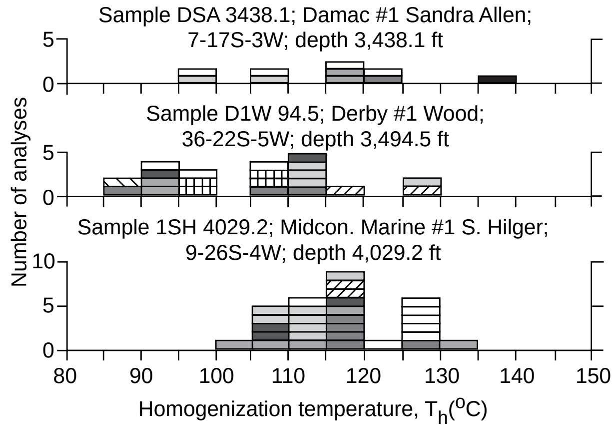
shaded.

FIGURE 10. Rock-Eval and vitrinite maturation profiles for two wells near McPherson County, Kansas (refer to fig. 8 for locations).

and Reynolds, 1994). In the case of the Viola Limestone, this temperature is estimated to be 115–130°C for both the Midcontinent Marine #1 South Hilger well and the Derby #1 Wood well, and 115–120°C for the Damac #1 Allen well. Although higher T_h measurements are recorded (fig. 11), they are either singular determinations or are from assemblages that have a broad temperature spread, making them less useful for estimating minimum temperature experienced by these rocks.

The T_h values are not corrected for pressure and therefore represent minimum temperatures of entrapment (Roedder, 1984; Goldstein and Reynolds, 1994). Even so, they are approximately 15–50°C greater than maximum temperatures inferred for the Viola Limestone based on its burial history and current geothermal gradients. The maximum recorded T_h of 139°C from a primary fluid inclusion at the Damac #1 Sandra Allen well (fig. 11) represents a temperature that is 49–69°C in excess of the maximum inferred burial temperature at the locality modeled in McPherson County (depending on what geothermal gradient is assumed). Even if the moderately “cool” temperature of 112°C (the average T_h from the Damac #1 Sandra Allen core) is conservatively taken as the maximum temperature experienced at that locality when the Viola Limestone was at its inferred maximum depth of 4,500 ft (1,370 m) during Late Pennsylvanian to Early Permian time, the resulting geothermal gradient would have to have been 68°C/km. This geothermal gradient is approximately twice the present-day gradient and is well in excess of any gradient that can be reasonably modeled from simple burial heating (fig. 3). If higher geothermal gradients are used, then calculated maturation unreasonably exceeds direct organic maturation or Cretaceous cover would have to be compensatorily unreasonably thin.

The uppermost modal T_h values will approximate a minimum estimate of how hot a mineral has been, either when it was precipitated, or particularly in the case of calcite, by subsequent reequilibration (Barker and Goldstein, 1990; Goldstein and Reynolds, 1994). The degree to which the highest modal T_h value approaches the actual maximum temperature is largely unclear though, due to ambiguities associated with pressure corrections, timing of entrapment, and other physical and chemical conditions affecting the inclusion (Goldstein and Reynolds, 1994). The highest modal T_h value of 125–130°C occurs in the Midcontinent Marine #1 South Hilger core, the most southerly and most deeply buried sample. However, the shallowest and most northerly sample from the Damac #1 Sandra Allen core does not record the lowest modal T_h value of all the samples analyzed. Its modal T_h of 115–120°C is 5°C greater than the modal T_h of the Derby #1 Wood well. There is no apparent correspondence between burial depth and modal T_h; therefore, a maturation model that invokes a linear increase in temperature with depth is probably not accurate to depict the burial and thermal history of the Viola Limestone. The temperatures recorded by the saddle dolomites probably represent one or more ephemeral thermal events: either one or more thermal pulses heating the entire stratigraphic column or advective fluid flow(s) out of the Ouachita foreland basin, as suggested by Leach and Rowan (1986).



Reflectance values for Ordovician strata are on vitrinite-like material. See text for discussion.

FIGURE 11. Histograms of T_h measurements, with fluid-inclusion assemblages noted, for samples of saddle dolomite from the Upper Ordovician Viola Formation from three cores in central Kansas (see fig. 1 for locations). Patterns indicate fluid inclusions from a single assemblage; blank indicates a single determination within a fluid-inclusion assemblage. The T_h values are well in excess of maximum burial temperatures inferred from TTI modeling. For a tabulation of these data, see Newell, 1996, table 8.7.

Summary and Conclusions

TTI modeling and organic maturation measurements generally indicate the Viola Limestone would be in initial stages of oil generation if it were a petroleum source rock. Theoretical maturation from TTI modeling can match maturation indicated by analyses of organic material, but constraints have to be placed on the interplay of the geothermal gradient and thickness of Cretaceous strata. Even when either of these two parameters are maximized though, the maximum expected burial temperature of the Viola Limestone falls well short of the temperatures indicated by T_h measurements, and patterns of T_h distribution and thermal maturation are inconsistent with assumptions of normal burial heating.

The geologic history of subsidence and uplift in the two localities modeled are fairly well constrained. If geologically unreasonable assumptions such as extreme geothermal gradients or excessive subsidence or uplift have to be invoked to achieve agreement with laboratory results, then chances are that the tectonic or geothermal inputs to the model are incorrect, or the modeling method itself may be too simple to model the actual situation presented by the maturation data. TTI models presented in this study implicitly assume the simple case of a constant geothermal gradient and vertical transfer of heat by conduction, and do not account for uneven heating of the stratigraphic column by heated brines. The poor fit of the maturation model to measured maturation indicates a different method of heat transfer may be likely.

A heat pulse, probably of short duration, appears necessary to account for the relatively high T_h measurements. A hint as to the nature of this heat pulse may lie in the depth profiles of the Rock-Eval and R_o measurements, and with the erratic distribution of T_h measurements with respect to their geographic distribution and depth. Organic-maturation parameters and maturation profiles in individual wells reveal well-to-well variations in maturation, erratic increases of maturation parameters with depth in individual wells, and even decreases of maturation with depth (figs. 8, 10). These anomalies indicate nonuniform heating of the rock column and temperatures that vary over short distances. Thermal anomalies may also be indicated by the homogenization temperatures of the saddle dolomites in that there is not a correspondence of greater T_h with depth. Although a thermal event is indicated by the fluid inclusions, even then the fluid inclusions do not necessarily have to record the maximum temperature experienced over the geologic history of these rocks, nor do the saddle dolomites necessarily have to be contemporaneous, so perhaps a good correlation of temperature with depth would be unusual.

Localized heating by vertical and lateral movement of formation waters may best account for these thermal anomalies and overall thermal maturity of the Viola Limestone. The most likely time for this fluid movement was probably during the Ouachita orogeny in late Paleozoic time inasmuch as this tectonic event had substantial structural effects inboard on the craton. Advective flow from the Ouachita orogen was shown by Wojcik et al. (1992, 1994) to affect Pennsylvanian strata in southeastern Kansas. Detailed work by Barker et al. (1992) and Walton et al. (1995) in the Cherokee basin of southeastern Kansas has also revealed marked spatial variations in maturation that indicate local "warm spots." These warm spots may have been formed by upward flow of warm waters through fractures into the Pennsylvanian section (Barker et al., 1992).

Heat transfer by movement of water onto the craton from peripheral orogens has been explained by a variety of processes. The efficacy of compaction (Cathles and Smith, 1983; Bethke, 1985; Hermanrud, 1986), tectonic compression (Oliver, 1986; Ge and Garven, 1989); topographic differences (Smith and Chapman, 1983; Garven and Freeze, 1984; Bethke, 1985; Bethke and Marshak, 1990; Deming et al., 1990; Deming and Nunn, 1991; Garven et al., 1993; Yao and Demicco, 1995) for long-distance movement of waters onto the craton have been quantitatively investigated, but more modeling will be needed. At present, compaction is possibly only of local importance (Cathles and Smith, 1983; Bethke, 1985; Hermanrud, 1986; Bethke et al., 1991). Thus the timing of significant fluid flow onto the craton and heating of the studied section may correspond to events during the Ouachita orogeny, possibly Pennsylvanian to Permian time (Oliver, 1986).

Further analyses of organic materials and fluid inclusions in saddle dolomites and related diagenetic minerals are needed to understand the spatial and stratigraphic pattern of the anomalous thermal event(s) in the midcontinent. Mapping and measuring these properties could help in understanding the process of fluid movement, as well as aid in ascertaining how orogenic events at the edge of the continental plates affect economic mineralization and petroleum migration on the craton inboard of the orogenic belt.

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