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Thermal maturity of the Swiss Molasse Basin: Indications for paleogeothermal anomalies? [1])

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Key Words: vitrinite reflectance, thermal modelling, fluid flow, foreland basin, Switzerland, Molasse

ABSTRACT

136 coal samples from outcrops of the Plateau Molasse and Subalpine Molasse of Switzerland have been collected in order to determine their maturation level and to reconstruct the thermal history during the Cenozoic. Measured mean random vitrinite reflectance values (Rr) range from 0.21% to 0.97%. Mean average values increase with age, from 0.39% Rr for samples from the middle Miocene OSM to 0.53% Rr for samples from the upper Oligocene USM, situated in the Plateau Molasse. Isoreflectance lines show a general increase in thermal maturity towards the Alpine front. Pronounced variations are found in the maturity values of the Plateau Molasse. Isoreflectance contours indicate that variations in thermal maturity might have a structural control. Areas of increased vitrinite reflectance occur near fault zones or lie parallel to a major topographic structure (Lake Zürich) which may be tectonically controlled. Thermal modelling of outcrop samples in the Plateau Molasse requires maximum paleotemperatures of about 40, 70, 90 and 110 °C for measured vitrinite reflectance values of 0.3, 0.4, 0.5 and 0.6% respectively. These temperatures could have occurred in a hypothermal peripheral foreland basin, if eroded overburden thicknesses of up to 4 km are assumed. However, there is no geological evidence for this amount of burial and consecutive uplift/erosion during the Neogene, especially in the distal parts of the Molasse basin. Thermal modelling, taking into account convective heat transport, could explain in part the inferred paleotemperatures and the observed coalification patterns. Zones of increased thermal maturation may, therefore, be related to an increased regional discharge of warm groundwater controlled by tectonic structures.

RESUME

Ce travail présente une étude de la maturation de la matière organique dans les sédiments de la Molasse du Plateau et de la Molasse subalpine en Suisse, et un essai de reconstitution de l'histoire thermique de l'avant-pays alpin au cours du Tertiaire. 136 échantillons de charbon ont été analysés. Leur pouvoir réflecteur moyen de la vitrinite (Rr) varie de 0.21% à 0.97%. La distribution de la réflectance de la vitrinite met en évidence un contrôle stratigraphique sur la maturation de la matière organique. Les valeurs moyennes varient de 0.39% Rr pour les échantillons de l'OSM à 0.53% Rr pour ceux de l'USM. Les courbes d'égal pouvoir réflecteur montrent une tendance régionale indiquant clairement une maturation croissante vers le front alpin. Cette tendance régionale est compliquée par des variations secondaires dans la Molasse du Plateau, qui semblent être liées à des accidents tectoniques. Ces derniers peuvent suivre les vallées principales (lac de Zürich). La modélisation thermique indique des paléotempératures maximales qui sont de l'ordre de 40, 70, 90 et 110 °C pour des valeurs de réflectance de la vitrinite de 0.3, 0.4, 0.5 et 0.6% respectivement. Admettant un paléogradient géothermique de 25 °C/km, on arrive à des valeurs d'enfouissement qui varient entre 1 et 4 km. Il y a, jusqu'à présent, aucun modèle géologique viable qui pourrait expliquer la sédimentation et l'érosion consécutive d'une couverture molassique si développée, surtout dans les parties distales du bassin. La modélisation thermique, avec un modèle qui inclut le transport de chaleur par convection, permet d'interpréter l'état de la maturation thermique du bassin molassique avec des valeurs

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d'enfouissement modestes (< 1 km). Les variations secondaires de la réflectance de la vitrinite pourraient être associées à des 'anomalies paléogéothermiques', dues à la remontée d'eaux chaudes dans des zones tectonisées.

1. Introduction

The geothermal regime in peripheral foreland basins is generally characterized as hypothermal, that is cooler than normal (Allen & Allen 1990; Robert 1985). The present thermal conditions of the Swiss Molasse basin indicate a low geothermal regime on a basin-wide scale. Geothermal gradients gradually decrease from > 35 °C/km close to the Rhine Graben in the North to < 25 °C/km towards the Alps (Rybach 1984). The present heat flow pattern is characterized by several positive anomalies in the eastern part of the basin and a more or less pronounced trend of decreasing values (100–60 mW/m^2) towards the Alps (Schweizerische Geophysikalische Kommission 1983).

Similar gradients are reported for the German Molasse basin (Vollmayr 1985). Teichmüller & Teichmüller (1986) interpreted the observed decrease of coalification gradients (0.09 to 0.03% Rm/km) in boreholes of the Bavarian Molasse towards the South as caused by a decrease of the geothermal gradient in the same direction. Such low gradients were prevailing since Late Miocene/Pliocene times.

The observed decrease in coalification and geothermal gradients in the North Alpine Foreland basin have been explained as a result of thickening of the crust towards the Alps (Teichmüller & Teichmüller 1986; Rybach 1984). Other important factors could influence the geothermal pattern in the Molasse basin:

i) The systematic variation of sediment thickness (increasing towards the Alps) and type of sediments (Molasse formations are coarser grained towards the Alps) could amplify the observed trend of the geothermal gradients. Rybach (1984) noticed that geothermal gradients are inversely proportional to the depth to basement.

An important controlling factor on the bulk thermal properties of sedimentary rocks is porosity, due to the differences in the thermal properties of the pore fluids and rock matrix. The specific heat capacity is much higher for water than for rocks (by a factor of about 5 to 1), whereas the thermal conductivity is lower. Therefore, the thermal conductivity of water saturated sediments may increase considerably during compaction.

Porosity in the Swiss Molasse basin seems to decrease towards the alpine front (Lemcke et al. 1968) due to cementation and/or increased burial. Assuming a conductivity dominated geothermal regime, such a porosity decrease should result in higher geothermal gradients towards the Alps. This is contrary to present day observations.

ii) Given the high heat capacity of water, geothermal gradient patterns are necessarily influenced by the hydrodynamic regime of a basin (Hitchon 1984; Lam et al. 1982). Recharge areas (topographic highs) are expected to display low geothermal gradients due to infiltration of cold surface water. Alternatively, regional topographic lows may display high geothermal gradients due to the discharge of warm water from depth and/or due to perturbations of the isotherms as a result of a topographic effect (e.g. river valleys). There is growing evidence that geothermal anomalies in sedimentary basins are often caused by uprising deep groundwater or other fluids, including water from the basement along highly permeable zones (Nesbitt 1990; Beck et al. 1989; Hitchon 1984). Deming et al. (1990) calculated that temperature perturbation resulting from possible fluid invasion can be as high as 50–150 °C. Cathles & Smith (1983) concluded that the relatively high temperatures (100–150 °C) at shallow depths (< 1.5 km) associated with the formation of Mississippi Valley-type lead-zinc deposits resulted from episodic dewatering, with brief pulses of hot brines carrying heat and dissolved solutes toward basin margins. Uprising deep groundwater is suggested as a cause of the present day heat flow anomaly (> 150 mW/m^2) in the distal part of the Molasse basin and the Jura ranges in Northern Switzerland (Rybach et al. 1987).

Few data have been published on the thermal maturity of the Swiss Molasse basin (Schegg 1991; Burkhard & Kalkreuth 1989; Monnier 1982; Rybach & Bodmer 1980; Kübler et al. 1979). Our knowledge of the burial history, paleogeothermal regime and the processes which control this regime is therefore quite incomplete. Indications of paleogeothermal anomalies are reported from the Western Molasse basin (Schegg 1991) and from the German Molasse basin (Jacob & Kuckelkorn 1977). They are probably linked to the paleohydrological regime.

The aim of this study is to determine the thermal maturity of sediments from the Swiss Molasse basin and to reconstruct it's thermal history during the Cenozoic [for an introduction to the geological setting of the Swiss Molasse basin see Homewood et al. (1986), Pfiffner (1986), Matter et al. (1980) and Trümpy (1980)].

Vitrinite reflectance (see Stach et al. 1982 for references) is a widely used parameter to estimate the degree of maturation of organic matter. Coal samples from the Plateau Molasse and Subalpine Molasse of Switzerland have been collected in order to:

- establish local and regional variations in vitrinite reflectance.
- examine the relationship between age and maturation of the major Molasse subdivisions (Lower Freshwater Molasse (USM), Upper Marine Molasse (OMM), Upper Freshwater Molasse (OSM).

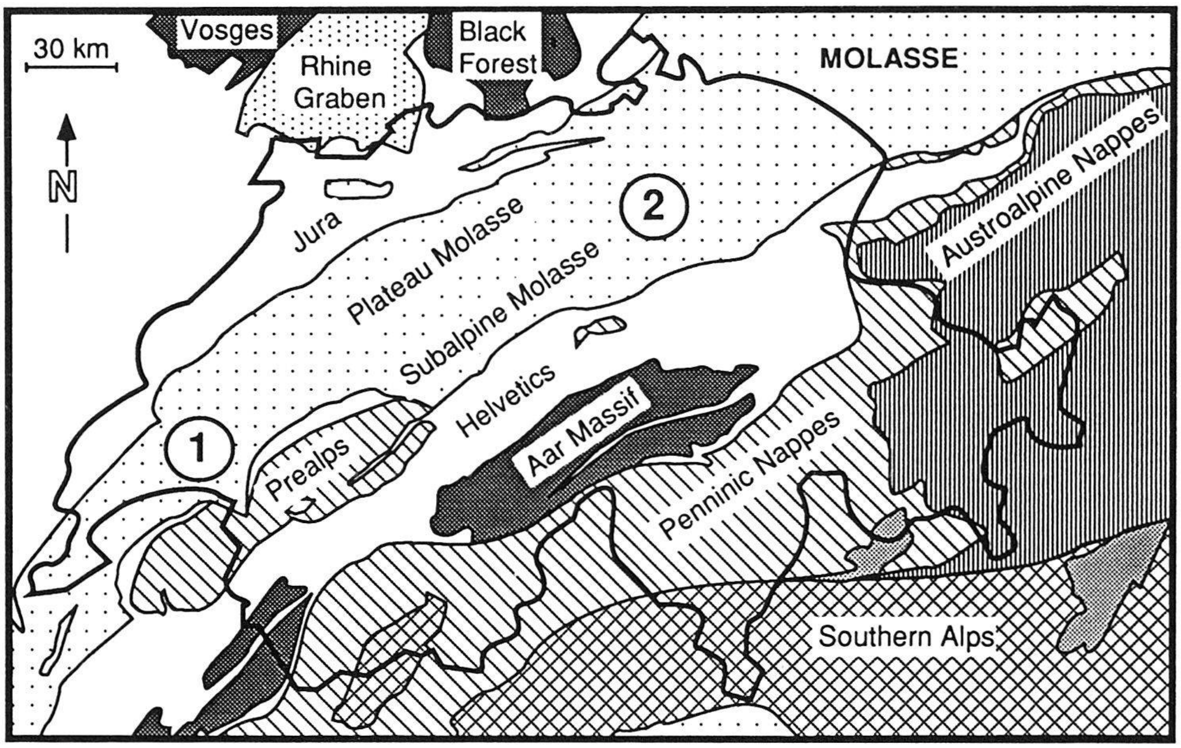

Fig. 1. Simplified tectonic map of Switzerland showing the study areas: 1 Gros-de-Vaud, 2 Eastern Switzerland.

Thermal modelling enables the estimation of the level of maturation for a given time-temperature history. It also provides important information, on the timing of maturation, on the causes of variation in maturation increases, and on the burial history of a basin (Sweeney & Burnham 1990; Larter 1989; Bustin et al. 1985; Waples 1980). The measured data will, therefore, be compared to expected values as obtained from model calculations.

In this study the regional pattern of vitrinite reflectance variation for the Gros-De-Vaud (Western Switzerland) and for Eastern Switzerland is outlined (Fig. 1).

2. Sampling and analytical method

136 coal samples from outcrops of the USM, the OMM and the OSM have been analyzed for this study.

In order to obtain the most reliable data on thermal maturation, only the vitrinite reflectance results of macroscopic coaly particles (branches, stems) and coal seams are included. Phytoclasts are most probably fragments of the woody material which was often washed into the sedimentary environment of the Molasse rocks.

The analysis of 5 shale samples from the Plateau Molasse containing abundant dispersed organic matter shows very high reflectance values (1.07–1.37% Rr) and a large scatter of the measurements. These observations indicate reworking of organic matter which was already coalified. This type of material was, therefore, not used for this study.

Surface samples will invariably be oxidized to some degree. According to Bustin et al. (1985), vitrinite reflectance of naturally oxidized coals is typically reduced. However, Marchioni (1983) found that low-rank coals show reflectance increase with increased weathering. The relative increase or decrease of vitrinite reflectance due to weathering can be up to 10% (Marchioni 1983). Therefore, small variations in vitrinite reflectance should be interpreted with care.

The coal samples were crushed to a particle size between 400 and 1000 μm, mounted in epoxy resin, then ground and polished with different diamond sprays (6, 3, 1, 0.25 μm). Mean random vitrinite reflectance (Rr) was determined using a Leitz MPV compact microscope under standardized conditions. The measurement procedure followed the rules outlined in the International Handbook of Coal Petrology (1971). The results were obtained from at least 50 measurements per sample.

3. Coalification data

The results of the vitrinite reflectance measurements are summarized in table 1. Reflectance values range from 0.21% Rr in a sample from the Upper Freshwater Molasse (OSM) of the Hörnli gravel fan in Eastern Switzerland, to 0.97% Rr in a sample from the Lower Freshwater Molasse (USM), situated in the Subalpine Molasse of Western Switzerland. The distribution of vitrinite reflectance values in the studied sedimentary formations (USM, OMM, OSM) clearly reveals that there is a stratigraphic control on maturation. Mean average values increase with age, from 0.39% Rr for samples from the middle Miocene OSM, to 0.53% Rr for samples from the upper Oligocene USM, situated in the Plateau Molasse. USM samples from the Subalpine Molasse show a slightly higher average (0.56% Rr).

	No	Location	X-Xoord.	Y-Coord.	Rr	S	N
GROS-DE-VAUD (Western Switzerland)							
Subalpine Molasse							
USM	RS10	Savigny	545900	154500	0,48	0,08	69
	RS11	Savigny	545900	154500	0,47	0,07	99
	RS280	Oron le Châtel	557230	158350	0,59	0,04	50
	RS281	Les Barattes	561640	162880	0,45	0,06	67
	RS283	Progens	559050	159090	0,37	0,04	50
	RS284	Bois du Riez	557520	161800	0,50	0,04	50
	RS353	Forêt de la Joux	560960	163780	0,47	0,05	50
	Weid10	Au Laviau / Jongny	554400	147900	0,76	0,07	100
	Weid12	La Gisetta	562800	161460	0,44	0,04	50
	Weid40	Jongny	554140	147670	0,51	0,05	51
	Weid41	La Conversion	541400	151800	0,48	0,07	70
	Weid42	Belmont	541700	152300	0,37	0,03	50
	Weid43	Rochettes	541200	151700	0,40	0,04	50
	Weid44	Mine de Progens	559200	159400	0,43	0,03	50
	Weid45	Mine de Bremont	560100	160280	0,52	0,05	50
	Weid47	Taborin	547400	153900	0,53	0,04	50
	Weid50	Mine de St.Martin	557700	158200	0,45	0,04	50
	Weid65	Moulin Monod	549080	147700	0,75	0,05	50
	Weid66	Jongny	554113	147560	0,65	0,07	50
	Weid67	Pont AR N9 sur Veveyse	555015	147509	0,81	0,04	50
	Weid68	Crau Coulet N9	547060	149610	0,56	0,03	50
	Weid70	AR N9, km 26.42	554950	147400	0,97	0,04	51
	Weid71	Tunnel de Belmont, AR N9	541940	152660	0,56	0,05	50
	Weid72	Tunnel de Belmont, AR N9	542000	152465	0,59	0,08	50
	Weid73	Tunnel de Belmont, AR N9	542000	152480	0,62	0,10	50
	Weid74	Les Brûlées	542640	151700	0,68	0,11	49
	Weid75	Tavernes, Coude de la Broye	552300	156500	0,63	0,07	50
	Weid77	La Biorde	553100	155390	0,49	0,06	53
	Weid79	Mine de la Conversion	541500	151500	0,41	0,04	50
	Weid81	Mine de Maracon	554850	156900	0,45	0,02	50
	Weid98	Mine d'Oron	553600	158000	0,46	0,04	50
	Weid99	Mine de Chattilens	552000	156900	0,52	0,05	50
	Weid100	Ruiss. de St.Amour	546700	154800	0,54	0,07	45
	Weid101	Crêt Rouge	546640	155360	0,59	0,07	70
	Weid102	Les Charbonnières	548700	156100	0,58	0,05	50
	Weid104	Parimbot	551900	161650	0,47	0,07	60
	Wi2036	Oron (VD)	552200	156400	0,67	0,12	100
	Wi2037	Oron	552200	156400	0,46	0,05	50
	Wi2038	Oron	552300	156450	0,43	0,05	50
	Wi2039	Les Thioleyres	552300	154675	0,36	0,05	103
Plateau Molasse							
USM	Weid1	Flon Morand	541870	155245	0,50	0,03	69
	Weid3	Talent 8	534620	168290	0,51	0,04	98
	Weid5	Talent 16	534810	168000	0,46	0,06	93
	Weid8	Talent 2	534880	170210	0,45	0,06	100
	Weid25	Ruiss. de Villarzel, Moulin des Anes	559640	178010	0,53	0,05	100

Table 1. Vitrinite reflectance data for the Swiss Molasse basin. Rr = mean vitrinite reflectance; S = standard deviation; N = number of measurements, Swiss coordinates used.

	No	Location	X-Xoord.	Y-Coord.	Rr	S	N
	Weid54	Sauvabelin	538850	153950	0,47	0,04	50
	Weid55	Prilly	536000	154000	0,47	0,04	50
	Weid56	Bois Mermet	537950	154200	0,57	0,05	50
	Weid57	Malley	536000	152900	0,45	0,05	50
	Weid58	Renens	535650	153775	0,46	0,02	50
	Weid59	Place du Tunnel à Lausanne	538400	153000	0,53	0,04	50
	Weid60	Place Chaudron à Lausanne	537600	152800	0,60	0,04	50
	Weid61	Place Chaudron à Lausanne	537600	152750	0,46	0,03	50
	Weid62	La Borde	538200	153300	0,54	0,04	50
	Weid63	Roveréaz	540900	153850	0,47	0,04	50
	Weid76	Venne, AR	539600	154800	0,49	0,04	50
	Weid85	Arrissoules	549280	183700	0,64	0,05	50
	Weid86	Ruiss. de la Croix	549700	183600	0,54	0,04	50
	Weid88	Bottens	540000	163000	0,51	0,04	50
	Weid89	Cuarny	542900	180100	0,52	0,04	50
	Weid91	La Mentue	543000	169000	0,43	0,02	50
	Weid92	Bavois, AR N1	533600	169600	0,40	0,02	50
	Weid95	Bavois	533200	170800	0,47	0,03	50
	Weid114	Talent 2	534880	170210	0,55	0,02	50
	Weid128	Chandelar-Flon Morand	540940	153830	0,46	0,03	49
OMM	RS325	Flon de Carrouge	550120	164970	0,51	0,04	50
	RS326	Broye	551680	165870	0,46	0,02	50
	RS351	La Neirigue	562450	167450	0,37	0,03	50
	Weid4	Ruisseau de Manloud	538960	156410	0,34	0,05	73
	Weid6	Flon Morand	542180	155635	0,45	0,04	99
	Weid7	Le Flon	540180	156220	0,36	0,03	100
	Weid13	Ruisseau des Losiardes (Lausanne)	542890	155210	0,44	0,02	49
	Weid14	Riau Gresin, pt. 605	551290	170420	0,42	0,04	99
	Weid15	Ruisseau de Lavaux-Morattel, pt564	560500	177950	0,43	0,05	100
	Weid16	Ruisseau de Planche-Roguin	561800	181440	0,43	0,05	69
	Weid17	La Neirigue	563565	170940	0,53	0,06	99
	Weid18	La Glâne, sur Châtel	566350	175760	0,49	0,07	70
	Weid19	Ruisseau de Seigneux, près 13 Cantons	556830	175050	0,55	0,05	100
	Weid20	Ruisseau de Colans	555400	171950	0,39	0,03	103
	Weid21	La Glâne, Moulin de Chénens	566280	176010	0,48	0,06	104
	Weid22	Ruisseau de Trey	560290	179780	0,55	0,04	50
	Weid23	Ruisseau des Vaux	555380	170810	0,48	0,05	100
	Weid24	La Trémeule	558210	176340	0,58	0,08	101
	Weid26	Chemin Seigneux - Les Granges	557060	174990	0,56	0,07	101
	Weid27	La Cerjaule, sous "Onze Malles"	551360	171770	0,48	0,06	50
	Weid29	La Cerjaule, sous les Envers	553035	173670	0,46	0,02	50
	Weid30	Le Recoulet, pt 631 Pissevache	552660	174560	0,39	0,03	50
	Weid31	Le Recoulet, pt 531	553340	173910	0,45	0,04	50
	Weid33	Ruiss. de la Chasse, Lucens	554950	174720	0,41	0,03	50
	Weid35	Ruiss. de Villeneuve	556260	177390	0,52	0,06	50
	Weid51	Grand Mont	538350	157150	0,53	0,05	50
	Weid53	Montenailles	539150	155600	0,51	0,03	30
	Weid82	Scierie de Croisettes	540800	155700	0,56	0,07	50
	Weid87	Le Flon, près Epalinges	540180	156240	0,48	0,06	50
	Weid105	Le Flon	552380	178160	0,43	0,03	50
	Weid111	Le Flon	552360	178440	0,38	0,04	50

	No	Location	X-Xoord.	Y-Coord.	Rr	S	N
	Weid123	Centrale / Lucens	553130	171520	0,47	0,03	50
	Weid127	Le Flonzel / Tour de St. Martin	547780	180810	0,41	0,04	50
	Weid126	Le Mausson / Grangettes	563600	169450	0,37	0,04	54
	Weid125	Le Flonzel / La Scie	547630	180060	0,40	0,02	50
	Weid124	Tour de la Molière	552910	183140	0,28	0,04	28
	Weid129	Carrière du Dézaley (Seiry)	554060	185270	0,41	0,05	50
EASTERN SWITZERLAND							
Subalpine Molasse							
USM	RS239	Mühlebachtobel (Greit)	691250	223750	0,58	0,05	50
	Weid52	Teufen	747000	251000	0,53	0,03	50
	Weid78	Bräun-Wanne	728935	229410	0,50	0,04	50
Plateau Molasse							
USM	RS209	Uznaberg	715150	232600	0,54	0,03	50
	RS210	Neuhüsler Tobel	714550	233800	0,47	0,03	50
	RS249	Zug	682100	223252	0,45	0,04	50
OMM	RS211	Echeltsschwil	715250	234750	0,44	0,04	50
	RS212	Curtiberg	708850	232850	0,42	0,04	50
	RS226	Mägenwil	660550	251075	0,44	0,04	50
	RS237	Ränggloch	660850	210100	0,50	0,03	60
	RS297	Hanenberg	661300	251150	0,40	0,05	50
	RS300	Mägenwil	659950	251050	0,52	0,04	50
	RS311	Würenlos	669650	255700	0,44	0,03	50
OSM	RS213	Ober Tägernau	708850	233350	0,44	0,02	50
	RS214	Bruederwald	715850	249600	0,35	0,03	50
	RS215	Bärtobel	712200	247500	0,38	0,05	50
	RS216	Bärtobel	712900	247800	0,25	0,04	40
	RS217	Leiachertobel	714150	246700	0,27	0,02	50
	RS218	Leiachertobel	713750	246550	0,36	0,04	50
	RS219	Chlihörnli	713440	248380	0,21	0,02	50
	RS220	Chlihörnli	713530	248300	0,31	0,04	50
	RS222	Fischbach	721600	277700	0,42	0,03	50
	RS238	Brunnentobel	682700	236150	0,37	0,03	50
	RS240	Kyburg	698000	256750	0,29	0,04	50
	RS241	Neuheim	687350	229575	0,36	0,02	50
	RS242a	Aeugst a. Albis	678800	237850	0,43	0,04	50
	RS242b	Aeugst a. Albis	678800	237850	0,47	0,08	50
	RS243	Schwizertobel	681700	238200	0,59	0,05	50
	RS244	Käpfnach (Stolleneingang)	688750	234550	0,48	0,02	50
	RS245	Käpfnach	688750	234550	0,54	0,05	50
	RS246	Brütten	693400	257950	0,48	0,04	50
	RS247	Baar	683675	227480	0,37	0,03	50
	RS248a	Pfefferberg	686600	232575	0,41	0,05	50
	RS248b	Pfefferberg	686600	232575	0,46	0,02	50

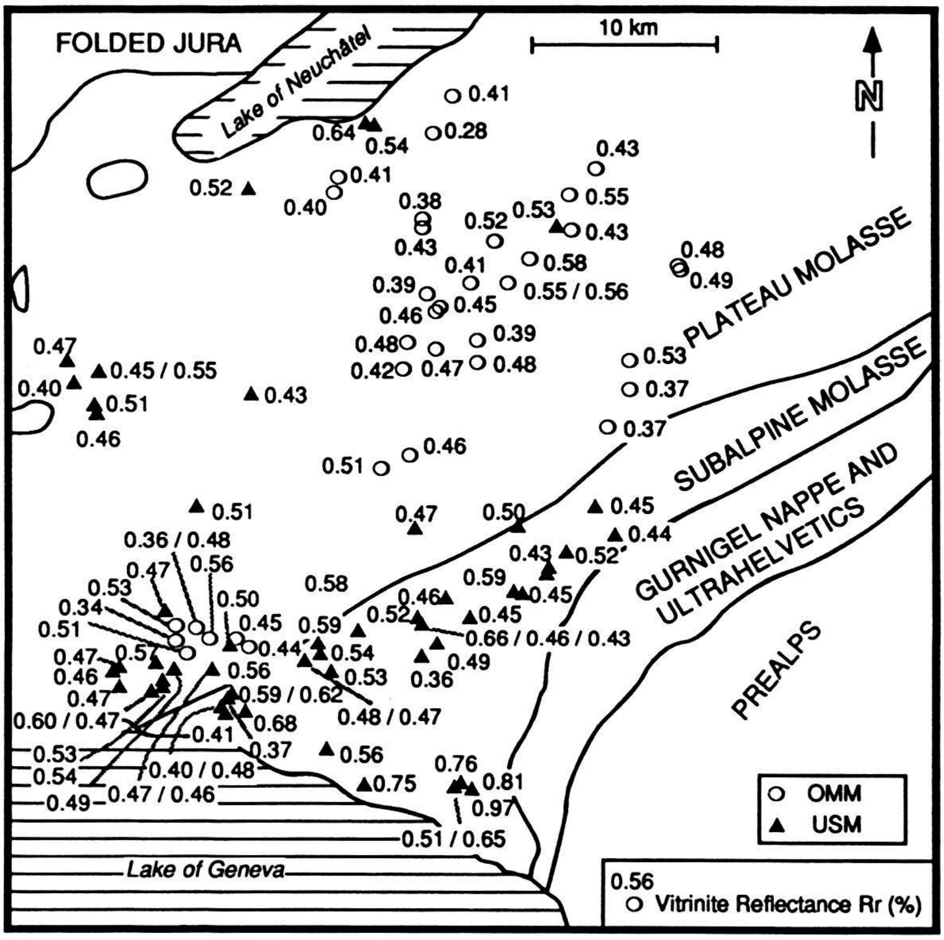

Fig. 2. Simplified tectonic map of Western Switzerland (Gros-De-Vaud) with mean vitrinite reflectance values from surface samples in the Molasse basin.

The thermal maturity of the coal samples varies also geographically. In order to represent this variation reflectance values were mapped and isoreflectance contours were calculated (by kriging). The limited number and uneven distribution of samples does not enable a unique interpretation. The chosen representation, nevertheless, shows the general trends and some interesting anomalies.

Gros-De-Vaud (Figs. 2 and 3):

The isoreflectance lines in the southern part of this area indicate an increase in maturity of the organic matter towards the Alps. This trend predominantly occurs in the Subalpine Molasse north of Lake Geneva. In the Plateau Molasse variations in vitrinite reflectance are rather sporadic. The most striking features are two limited regions with relatively high maturity levels (Rr > 0.5%). One zone is situated just south of Lake Neuchâtel. It is interesting to note that the three analyzed samples in this region are lying along the Pomy-Cuarny thrust (PC in Fig. 3). Another area of increased thermal maturity is situated about 10 km southeast of Lake Neuchâtel, in the La Broye valley, where values of up to 0.58% Rr were measured. Again a major thrust (Sarens-Les-Granges, SLG in Fig. 3) is located close to this zone.

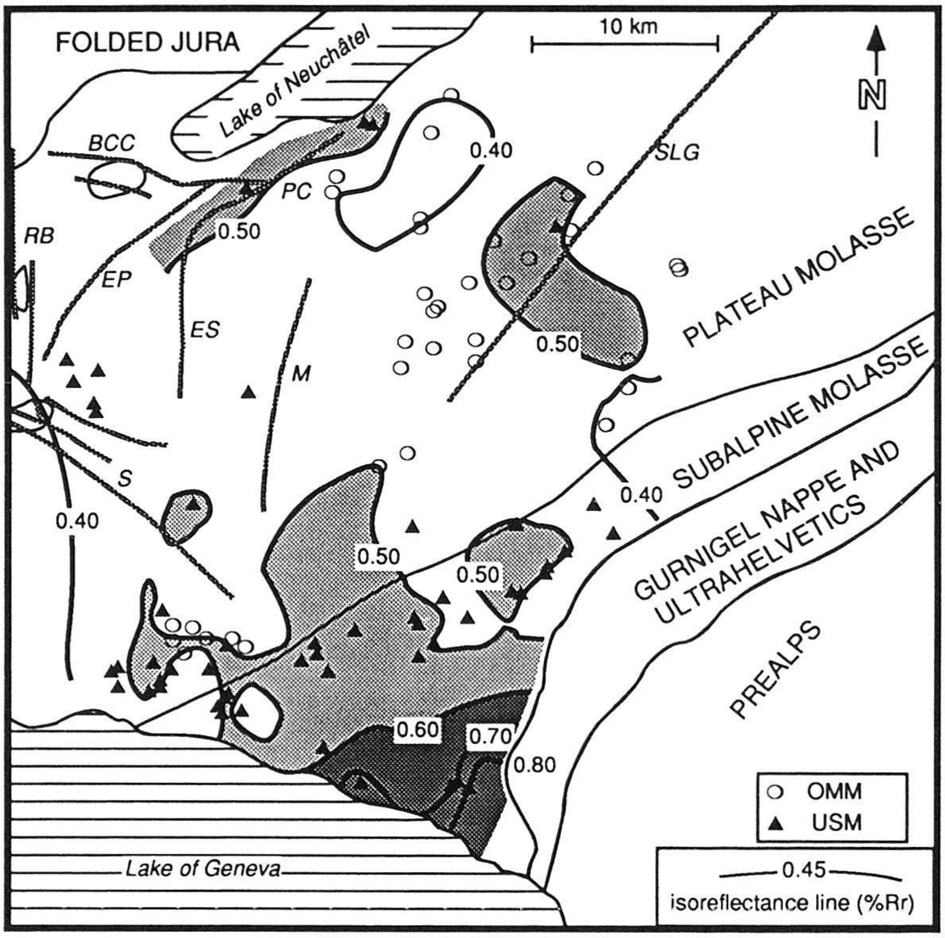

Fig. 3. Isoreflectance map of Western Switzerland. Interpretation of mean vitrinite reflectance values by kriging. The isoreflectance lines indicate an increase in maturity of organic matter towards the Alps. There are, however, zones of increased thermal maturity (Rr > 0.5%) in the Plateau Molasse. Tectonic structures are modified from Jordi (1990): BCC = Baulmes-Chamblon-Chevressy thrust, ES = Essertines fault, EP = Ependes fault, M = Mentue thrust, PC = Pomy-Cuarny thrust, RB = Rances-Baulmes fault, S = La Sarraz fault, SLG = Sarens-Les-Granges thrust.

Eastern Switzerland (Figs. 4 and 5):

Despite a limited number of samples in this area, some general trends are clearly observed. Isoreflectance lines show a general increase in thermal maturation towards the Alpine front. This pattern is disturbed by an area of increased vitrinite reflectance running parallel to Lake Zürich. Samples from the distal part of the Plateau Molasse (between the eastern termination of the folded Jura and Zürich) display surprisingly high maturity values (0.40–0.52% Rr).

4. Thermal modelling

a) Theoretical Considerations

Vitrinite reflectance is a widely used indicator of thermal maturity in oil and gas exploration (Tissot et al. 1987; Tissot & Welte 1984), and regarded as the most reliable and precise method for quantifying organic diagenesis (Bustin et al. 1985). It is recog-

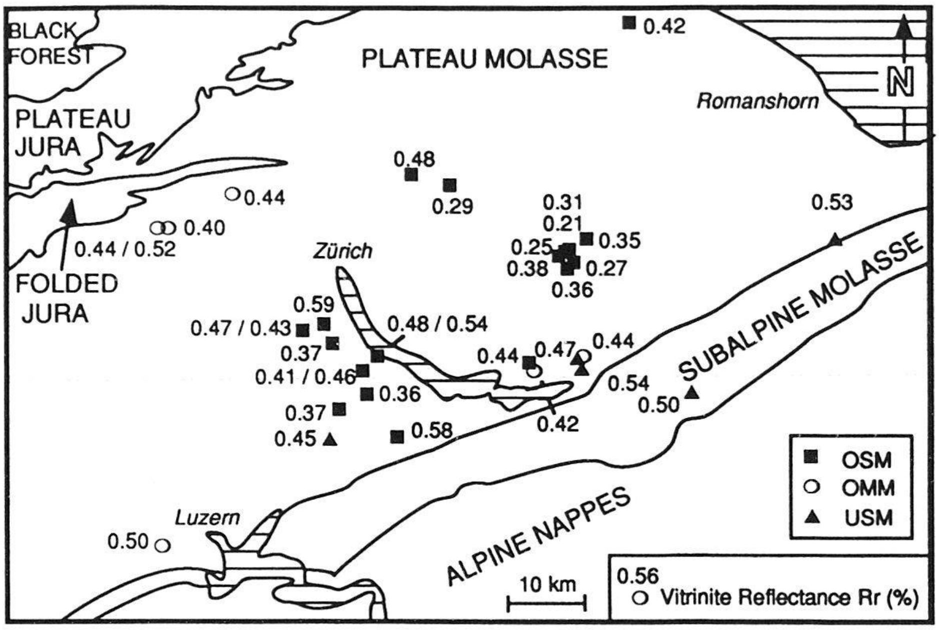

Fig. 4. Simplified tectonic map of Eastern Switzerland with mean vitrinite reflectance values from surface samples in the Molasse basin.

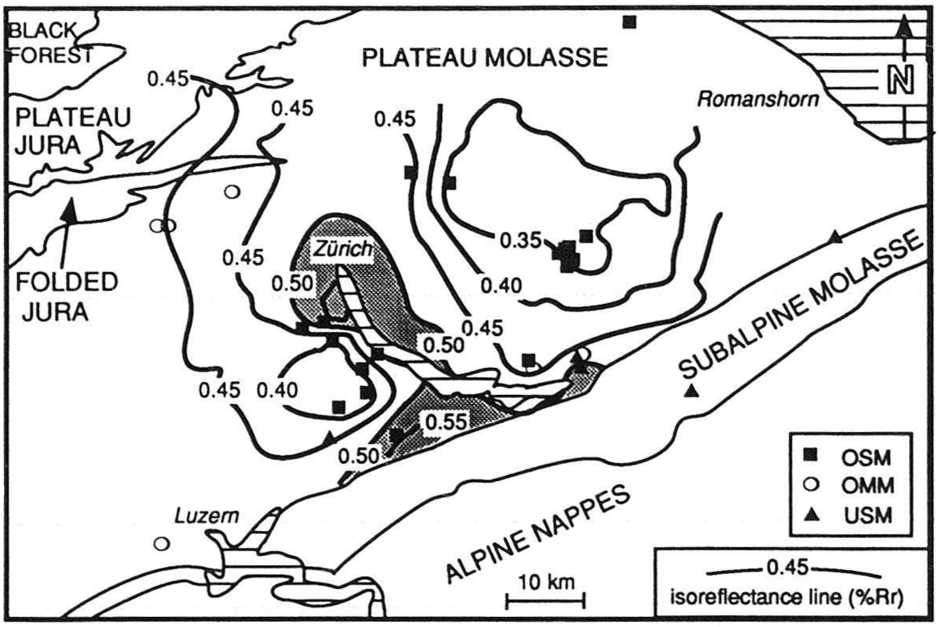

Fig. 5. Isoreflectance map of Eastern Switzerland. Interpretation of mean vitrinite reflectance values by kriging. The isoreflectance lines indicate an increase in maturation of organic matter towards the Alps. A zone of increased thermal maturity running parallel to the Lake of Zürich disturbs this simple pattern.

nized that the rank of coal, normally defined by vitrinite reflectance, is mainly a function of temperature and time (Karweil 1956). Therefore, vitrinite reflectance and other maturation indices of organic matter (Carbon Preference Index, C.P.I., Thermal Alteration Index, T.A.I. ...) cannot be directly converted to paleotemperature. All indices of organic diagenesis are a function of the thermal history through rather complex kinetics which are frequently influenced by the type of organic matter (Tissot et al. 1987).

A popular and simple approach for quantifying organic diagenesis was developed by Lopatin (1971). This method calculates a maturation parameter by the integration of the entire time-temperature history of a stratum assuming that increasing the temperature by 10 °C doubles the maturation reaction rate. A modified version of Lopatin's method which correlates a calculated maturation parameter (TTI = temperature time index) with vitrinite reflectance was published by Waples (1980). These approaches have been criticized because the effect of the duration of heating on the thermal maturation of sedimentary organic matter seems limited (Barker 1983; Price 1983). According to Barker (1989), organic matter stabilizes with respect to temperature after about 10^6 to 10^7 years in burial diagenesis, 10^4 years in geothermal systems and about 10^{-1} to 10^0 years in contact metamorphism by intrusive sheets. The assumption that the rate of maturation doubles every 10 °C is considered to be inaccurate (Burnham & Sweeney 1989). With the actual activation energies of kerogen transformation reactions (45–65 kcal/mole), doubling the reaction time is equivalent to a temperature increase of 3–5 °C (Tissot et al. 1987). Accordingly the Lopatin-Waples calculations tend to underestimate thermal maturity at high heating rates (rapid burial) and overestimate it at low heating rates (Wood 1988).

More recently the development of kinetic models for vitrinite reflectance evolution, based on viable chemical principles, provide new tools for thermal modelling (Sweeney 1990; Sweeney & Burnham 1990; Larter 1989). These models are based on the classical formulation of first-order kinetics, which are also applicable to the degradation of kerogen. An important aspect is the consideration of several parallel reactions which accounts for the diversity of composition and distribution of chemical bond types in the original kerogen (Tissot et al. 1987).

b) Modelling Strategy

For the reconstruction of the thermal history, an iteration process is used. The combination of the structural history (burial vs. time) and a first simplified thermal history (geothermal gradient vs. time) results in a temperature history. By mathematical modelling, the evolution of kerogen and related maturity indices can be obtained. The comparison of modelled and measured maturity indices allows to adjust progressively the parameters which determine the thermal history.

There is growing evidence that the paleogeothermal regime of sedimentary basins is influenced by the paleogeohydrological conditions (Beck et al. 1989; Oliver 1986). The thermal regime of a sedimentary basin may be influenced by factors such as the hydraulic conductivity, density and viscosity of water, basin geometry, topography, water-table configuration, thermal conductivity, geothermal heat flow and climate (Garven & Freeze 1984). Many of these parameters change in time and space and obviously heat flow values and/or geothermal gradients will be directly affected by these variations.

Two different approaches are chosen for this study. 1) The "burial history approach" assumes that the temperature history of a formation mainly depends on the burial depth. The thermal conditions are governed by constant relatively low geothermal gradients and low heat flow values. There is a slow increase in temperature during burial and a decrease during erosion. 2) The "geohydrological approach" is based on a modified burial history.

This approach assumes varying geothermal gradients (both in time and depth) due to changing paleogeohydrological conditions. Rapid changes in temperature for short time periods could be expected with an influx of hot (or cold) water.

c) "Burial History Approach"

The EASY % Ro-model of Sweeney & Burnham (1990) was used for this study. This model uses an Arrhenius first-order parallel reaction approach with a distribution of activation energy. It enables the calculation of the vitrinite maturation history (% Rr versus time) for a given temperature history (temperature versus time) and applies to values of mean random vitrinite reflectance from 0.3–4.5 % Rr.

The maturation history for two time horizons corresponding to the base of the USM and the OMM (30 my and 20 my) in the Plateau Molasse was calculated. The modelled final (present-day) values are compared to the measured values of outcrop samples.

In order to constrain the thermal history, the following assumptions are made:

- The mean annual surface temperature is estimated at 20 °C during the Oligocene and Miocene. This is a rather conservative value as palynological investigations (Hochuli 1978) suggest temperatures of 15–18 °C during the Oligocene. Present day values are at 10 °C.
- Maximum paleodepths were reached toward the end of the middle Miocene (12 my). This is marked by the end of Molasse sedimentation and the start of uplift and erosion (Pfiffner 1986; Mugnier & Menard 1986; Naef et al. 1985; Lemcke 1974). The start of the uplift history is set at 12 my, although thrusting and uplift in more internal parts of the basin (Subalpine Molasse) probably took place earlier (Burkhard & Kalkreuth 1989).
- The temperature increase of a time horizon is only dependent on the burial history.

Temperature histories with maximum paleotemperatures, varying from 40 to 160 °C, are used to model final (present day) maturation values for each time horizon. Figure 6 shows a diagram of calculated vitrinite reflectance values (% Rr) versus maximum paleotemperatures (Tmax). The plot clearly indicates that time "plays" only a minor role. Measured vitrinite reflectance values of outcrop samples in the Plateau Molasse range from 0.2 to 0.6 % Rr. Modelling shows that this would correspond to maximum paleotemperatures of up to 110 °C. With an assumed average paleogeothermal gradient of 25 °C/km paleodepths of up to 4 km would be required to explain these vitrinite reflectance values from surface samples. This is much more than expected from the overlaying stratigraphic column, almost entirely preserved in the eastern part of the Swiss Molasse basin. The thickness of sediments, overlying analyzed outcrop samples (e.g. OMM and OSM), may have extended to 2 km in the most proximal part of the basin. In the distal parts, however, this overburden thickness decreases to some hundred meters (Matter et al. 1980).

The zone of increased thermal maturity in the La Broye valley (Figs. 2 and 3) shows vitrinite reflectance values of 0.52–0.58 %. This is an increase of over 0.1 % Rr when compared to the average values from the surrounding area. In terms of maximum paleotemperatures, an increase of about 30 °C is suggested by these calculations.

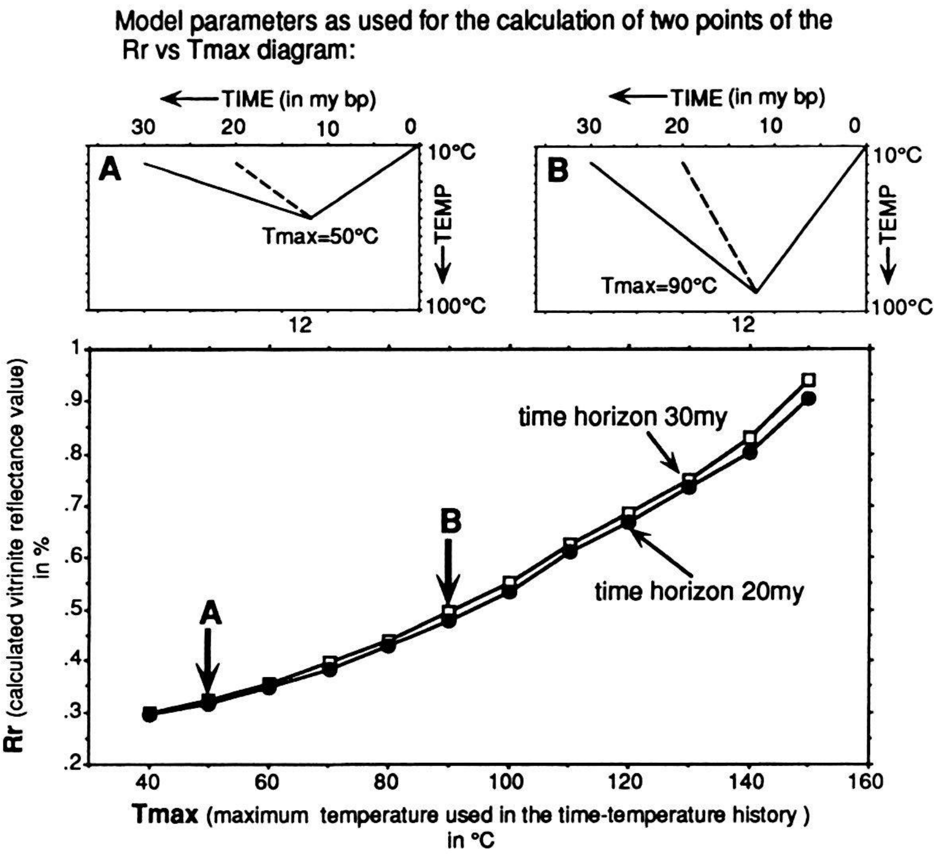

Fig. 6. Thermal modelling with the EASY % Ro model of Sweeney & Burnham (1990) enables the calculation of mean vitrinite reflectance values (Rr) during time for a given stratigraphic level if the time-temperature history is known. The final Rr-values of two different time horizons for changing temperature histories are plotted on a Rr vs. Tmax (maximum paleotemperature for each temperature history) graph.

d) *"Geohydrological Approach"*

This approach uses a conceptual framework different to that used in the burial history approach. It is probably a speculative model. However, its aim is to show that the observed coalification pattern could be modelled without the requirement of a high amount of erosion in a generally low-temperature regime. The latter is typical for the Molasse basin.

Since only outcrop samples are analyzed in this study, modelling results would have to be calibrated with only one measured vitrinite reflectance value. This is probably not a very reliable approach. For this reason published vitrinite reflectance data from the Küsnacht drillhole are used (Rybach & Bodmer 1980) to calibrate the geohydrological approach. As in other wells of the Molasse basin (Teichmüller & Teichmüller 1986), there is a low coalification gradient (0.08 % Rm/km) indicating a low paleogeothermal gradient.

For the construction of the burial history curves, the amount of the eroded section has been set to a value of 1 km. This is higher than assumed erosion estimates for this region (Naef et al. 1985; Laubscher 1974; Lemcke 1974), but lower than estimates of the burial history approach or of a recent study on rock density and compaction in the Swiss

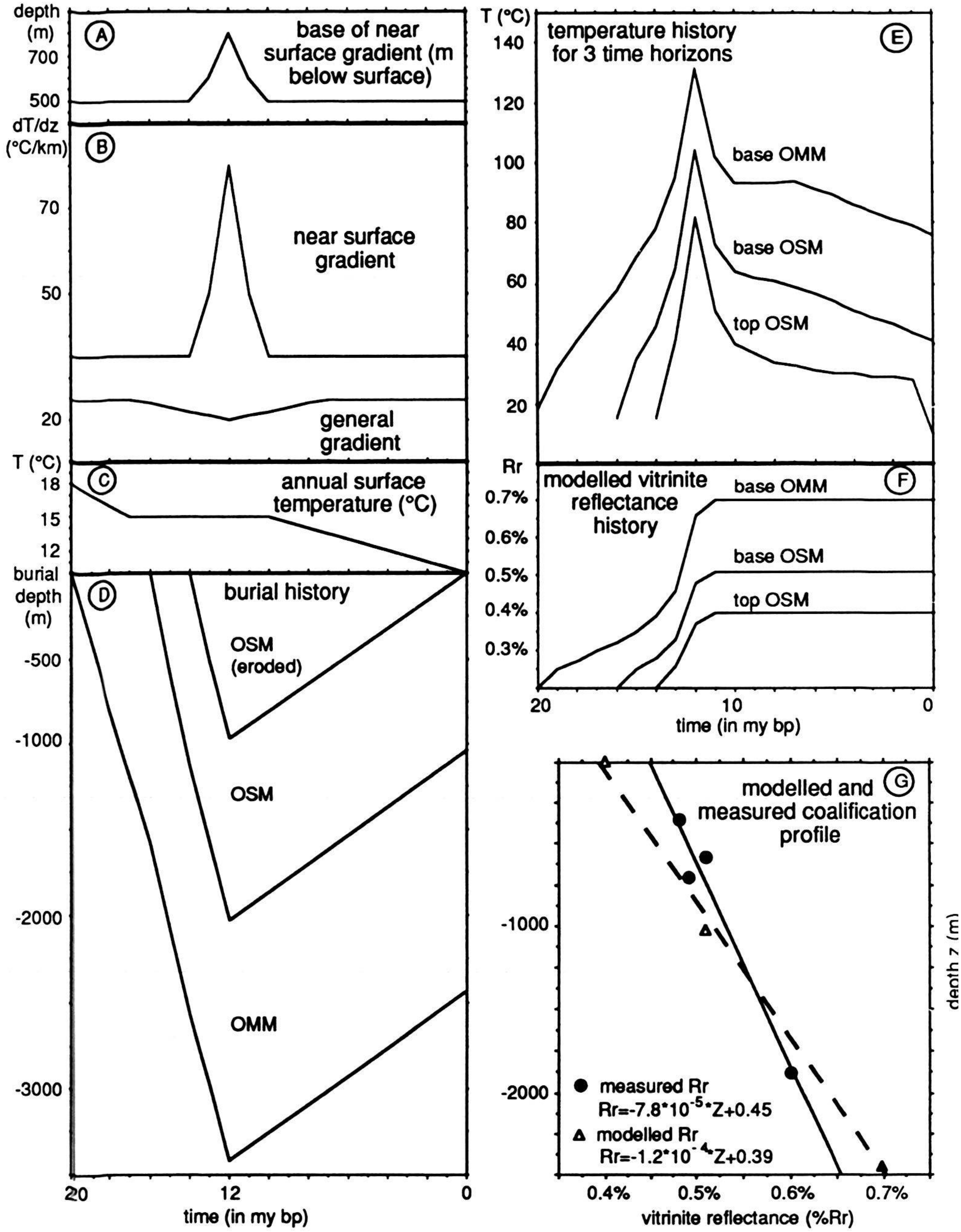

Fig. 7. Thermal modelling of data from the Küsnacht well with the EASY % Ro model (Sweeney & Burnham 1990) and a conceptual model which takes into account hypothetical effects of convective heat transport ('geohydrological approach'). The variation of different input parameters (A – D) enables the calculation of time-temperature histories (E). Using the EASY % Ro model these temperature histories can be 'transformed' into maturity histories (F). (G) shows the comparison between modelled and measured coalification profile.

Molasse basin (Kälin et al. 1992). The latter study indicated very high values of about 4 km, unaccounted for by any geological observation.

The present day geothermal gradient pattern of the Swiss Molasse basin (Rybach et al. 1987; Vollmayr 1983) is characterized by a rapid increase of temperature near the surface (30–60 °C/km, < 500 m). This high near-surface gradient could be due to convective heat transport by groundwater (Rybach & Bodmer 1980). Although there are no indications yet, it is probable that the thermal gradient and depth of this zone could have changed in time and space. This may be the result of a change in the fluid flow pattern in the Molasse basin due to:

- a variation of the topography.
- fluids tectonically expelled from the orogenic belt.
- climatic variations influencing the infiltration rate of recharge areas (Balderer 1990).
- a variation of the groundwater interface (surface separating low mineralized groundwater of Na-HCO_3-type above and strongly mineralized groundwater of Na-Cl-type below) observed within the deeper and central part of the Molasse basin (Balderer 1990).

Figure 7 presents the input parameters and resulting temperature as well as maturity values of a successful simulation. The main assumptions are a deepening of the base and an increase in the near surface gradient value at the time of maximum burial. This variation (probably due to increased convective heat transport) could be caused in part by the high relief of the Alps during the Early and Middle Miocene (Pfiffner 1986). The combination of the burial history (Fig. 7D) and the variation of the mentioned thermal parameters (Fig. 7A–C) enables the calculation of the temperature history (Fig. 7E) for certain time horizons. Using the EASY% Ro-model, these temperature histories can be 'transformed' into maturity histories (Fig. 7F). The comparison between the modelled and measured coalification profile of the Küsnacht drillhole (Fig. 7G) indicates a 'good fit'.

5. Implications for the paleogeothermal regime of the Molasse basin

The main features resulting from the vitrinite reflectance analysis and thermal modelling can be summarized as follows:

i) Pronounced variations are found in the maturity values from outcrop samples of the Plateau Molasse (0.21%–0.64% Rr).

ii) Isoreflectance contours indicate that variations in thermal maturation might have a structural control. Areas of increased vitrinite reflectance occur near fault zones or lie parallel to a major topographic structure (Lake Zürich) which may be tectonically controlled (Hantke 1967).

iii) The degree of thermal maturity in the Plateau Molasse, especially in the Gros-De-Vaud area and west of Lake Zürich, is higher than expected. A region of low thermal maturity can be observed east of Lake Zürich (Hörnli area).

iv) Maturity of organic matter generally increases towards the Alps.

v) Thermal modelling of outcrop samples in the Plateau Molasse requires maximum paleotemperatures of about 40, 70, 90 and 110 °C for measured vitrinite reflectance values of 0.3, 0.4, 0.5 and 0.6% respectively.

vi) The Küsnacht drillhole (Rybach & Bodmer 1980) is characterized by a low coalification gradient and a high degree of maturity at shallow depth (0.48% Rr at 350 m). When modelling with a classical burial history approach, a considerable amount of erosion (3–4 km) is needed to calibrate the calculated data. Alternatively, the high Rr values and the low geothermal gradient could both be explained by a short-time discharge of warm groundwater in this region. The magnitude of erosion (1 km) resulting from such a simulation corresponds with values given in the literature (Naef et al. 1985; Laubscher 1974; Lemcke 1974).

Maturation patterns at the surface of the Swiss Molasse basin are mainly determined by the individual thermal history of each sample site. Many, partly interrelated, parameters are influential: sedimentary and/or tectonic overburden, local uplift/erosion, heat flow at the base of the Molasse basin, convective heat transport (fluids expelled from the orogenic belt, rising deep groundwater in fracture zones, gravity-driven fluid flow), long term changes in surface temperature, sedimentation rate, topography and the geometry of the formations.

Conventionally, maximum burial depth is regarded as the most important factor for coalification in hypothermal basins. The decollement induced uplift of the Molasse basin increases from several hundred meters in the north and east to over 2000 m in the southwest (Laubscher 1974; Lemcke 1974). Monnier (1982) in a study of clay mineral diagenesis confirmed these conclusions.

Thermal modelling indicates maximum paleotemperatures of up to 110 °C for surface samples in the Plateau Molasse. In Northern Switzerland the paleotemperature would be between 70 and 90 °C. Relatively high temperatures during the Tertiary are in part confirmed by a fluid inclusion study of Tertiary, Mesozoic and Permo-Carboniferous sedimentary rocks from several boreholes of Northern Switzerland (Mullis 1987). For one group of inclusions ("late salt-poor inclusions") which were probably formed during the Miocene, trapping temperatures between 70 and 140 °C were measured.

These temperatures may be easily interpreted in the context of a low geothermal regime, if the results of the burial history approach (chapter 4c) or the results of a recent study (Kälin et al. 1992) on rock density and compaction in the Plateau Molasse (indicating eroded overburden thicknesses of up to 4 km) were confirmed. However, there is no geological evidence for large amounts of burial and consecutive uplift/erosion during the Neogene (Laubscher 1987, 1974; Naef et al. 1985), especially in distal parts of the Molasse basin. Furthermore, no viable tectonic concept explains the accumulation and subsequent removal of an additional 4 km of sediments during the Middle Miocene on the Plateau Molasse.

Convective heat transport may partially explain the inferred paleotemperatures and the observed coalification pattern. There is some independent evidence for this interpretation:

i) The present day heat flow anomaly in Northern Switzerland, explained by uprising deep groundwater (Rybach et al. 1987), shows that convective heat transport is important for the present geothermal regime of the Molasse basin.

ii) Within the present day heat flow pattern of the Swiss Molasse basin geothermal anomalies are not an isolated phenomena.

iii) Second order variations in the coalification pattern of the investigated areas can not be explained only as the result of locally very high overburden-thicknesses and high uplift/erosion values. These small scale anomalies, which may be structurally controlled, probably resulted from the regional discharge of warm fluids.

Similar phenomena have been postulated elsewhere: Clendenin & Duane (1990) confirmed a tectonic link between the Appalachian-Ouachita orogeny and the Mississippi Valley-type Pb-Zn deposits of its foreland basin. Seismic pumping and distal fluid focusing along faults appeared to be a plausible mechanism to move hot reactive fluids to the sites of ore deposition. Thermal anomalies could also be explained by a gravity-driven fluid flow (Hitchon 1984) which is controlled by high permeable fault zones or rising deep ground water in fracture zones.

iv) If the level of maturation is influenced only by the overburden-thicknesses, a decrease in maturation from the west to the east should be observed, since erosion has cut much deeper into the Western Molasse basin than in the east. However, this relationship is not revealed by our data. Vitrinite reflectance values west or north of Zürich are the same as in Western Switzerland. This supports the hypothesis that the thermal regime of the Molasse basin is influenced by other factors in addition to the overburden thicknesses.

v) Thermal modelling, assuming some hypothetical effects of convective heat transport, can successfully simulate low-gradient coalification profiles with a low overburden-thickness.

vi) Similar paleogeothermal anomalies are reported from the Western Molasse Basin (Schegg 1991). A hydrothermal influence is also proposed for an important maturity anomaly (Rr of up to 1.3% at a depth of only 3100 m) in the Miesbach 1 well in Bavaria (Jacob & Kuckelkorn 1977).

The influence of the paleogeohydrological system on the paleogeothermal regime of the Molasse basin has been underestimated in the past. Nevertheless, burial depth is a very important parameter to interpret coalification patterns. The increase of thermal maturity towards the Alps is probably a consequence of increasing burial depth towards the orogenic belt.

6. Conclusions

The results of this study show that different relationships exist between the very low-temperature metamorphism in the Molasse basin and the tectonic history of the adjacent Alps.

Increasing burial of Molasse sediments towards the Alps is indicated by the general increase of thermal maturity in the same direction.

The coalification pattern of the Plateau Molasse supports the hypothesis that the paleogeohydrological system "played" an important role for the paleogeothermal history of the Molasse basin. Zones of increased thermal maturation may therefore be related to a regional discharge of warm groundwater controlled by tectonic structures.

The level of maturation at the surface in the Plateau Molasse basin is rather high (up to 0.64% Rr). Conventionally, in hypothermal basins this would be explained by a thick overburden. The results of this study indicate, however, that the observed thermal maturity may be due to a combination of 'not-so-deep' burial and transient heating by warm fluids.

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