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Predicting methane accumulations generated from humic carboniferous coals in the Donbas fold belt (Ukraine)

Dani Alsaab, Marcel Elie, Alain Izart, Reinhard F. Sachsenhofer, and Vitaliy A. Privalov

ABSTRACT

The numerical modeling of the Ukrainian part of the Donbas fold belt indicates that the coalification pattern was controlled mainly by the maximum burial depth of coal seams and the heat flow (HF) (40–75 mW/m^2) during the Permian. The coalification pattern was overprinted by magmatic events during the Late Permian in the south syncline (150 mW/m^2) and during the Permian–Triassic in the north of the Krasnoarmeisk region (120 mW/m^2). The coalification pattern shows a strong increase in vitrinite reflectance values toward the east and southeastern parts of the study area likely caused by (1) an eastward increase in burial depth, (2) a probable eastward increase in HF, and, (3) probable magmatic activity. An increase in total erosion toward the eastern and southeastern parts was also observed with a maximum erosional amount of approximately 8 km (5 mi) in the southeastern part of the study area. The basin modeling of this area predicts that the main phase of hydrocarbon generation occurred during the Carboniferous–Early Permian subsidence. The magmatic events that occurred during the Permian–Triassic caused renewed pulses of hydrocarbon generation. A large amount of the generated hydrocarbons was lost to the surface because of a lack of seals. However, the numerical simulation predicts accumulations of about 2 tcf (57 billion m^3) of methane generated from Carboniferous coals in the south and main synclines, where Lower Permian seal rocks are preserved. Finally, this study provides data on methane resources along the northern flank

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of the basin, which remains a significant frontier for natural gas exploration.

INTRODUCTION

The Dniepr-Donets Basin (DDB) in Ukraine is an important hydrocarbon province (Ulmishek et al., 1994; Chebanenko et al., 1995; Kabyshev et al. 1998; Ulmishek, 2001). This basin experienced inversion movements, uplifts, and erosions that were more intense to the southeast through geologic time (Chekunov, 1976; Chekunov et al., 1992; Stovba et al., 1996; Privalov, 1998; Stovba and Stephenson, 1999; Saintot et al., 2003a, b; Stephenson et al., 2006). The Donbas fold belt (DF) is the strongly inverted and deformed part of the DDB covering an area of 60,000 km^2 (23,166 mi) in the southeastern part of Ukraine and adjoining areas in Russia. The deformed strata mainly consist of Carboniferous with, however, Lower Permian sediments preserved along the northwestern margin of the basin (Popov, 1966; Stovba and Stephenson, 1999).

The DF contains some of the world's most important coal resources in terms of quantity and quality (Sachsenhofer et al., 2002; Privalov et al. 2004a). However, conventional gas deposits are known in structural traps sealed by Lower Permian rocks along the northern margin of the DF (Privalov et al., 2007). Mississippian and Lower Permian clastic rocks, and at a much lesser level the carbonates, are the main reservoir lithologies (Ulmishek et al., 1994; Kabyshev et al., 1998; Ulmishek, 2001). Basin inversion, uplifts, and subsequent erosions of sedimentary layers, especially Lower Permian salt-bearing sequences, within the DF may have induced the vertical migration and loss of hydrocarbons to the surface. However, the DF contains viable prospective sites for conventional and coalbed methane accumulations in the Carboniferous coal-bearing strata. The potential resources have been estimated to be in the range of 12–27 trillion m^3 (424–953 tcf) (Uziyuk et al., 2001; Privalov et al., 2004b). Triplett et al. (2001) estimated the coalbed methane resources to be 1.4–2.5 trillion m^3 (49–88 tcf) in mineable coal seams. Deposits in cupola-like structures related with dextral strike-slip zones along the northern marginal fault of the DF host conventional gas reserves of 240 billion m^3 (8500 bcf) (Privalov et al., 2007).

The Pennsylvanian marine shales and carbonates are considered as principal source rock intervals for the Dniepr-Donets hydrocarbon system formation, although the function of the Carboniferous coals is still uncertain (Ulmishek et al., 1994; Ulmishek, 2001; Privalov et al., 2005; Ivanova, 2006).

However, Carboniferous humic coals from the DF, mostly rich in collodetrinite and liptinite (sporinite and alginite), holding a hydrogen index (HI) of 200–300 mg HC/g total organic content (TOC) (Sachsenhofer et al., 2003), and containing long aliphatic chains higher than C_{18} (Alsaab et al., 2007), can be regarded as oil- and gas-prone source rocks (Bertrand, 1984; Wilkins and George, 2002, and references therein; Privalov et al., 2007). Considerable work was conducted to understand the relationship between the coalification pattern and the effects of magmatic bodies, tectonic events, HF history, and erosional processes in the DF (Porfiriev, 1948; Triplett et al., 2001; Uziyuk et al., 2001; Sachsenhofer et al., 2002; Privalov et al., 2003, 2004a, b). To date, no detailed two-dimensional (2-D) modeling study has been performed on this basin. Consequently, the key factors controlling the generation, migration, and accumulation of hydrocarbons are poorly constrained. In addition, the thermal history in the northern flank of the DF has not been studied before.

In this article, the numerical simulation of the DF was performed and calibrated with more than 40 wells along 6 cross sections in the Krasnoarmeisk, Donetsk, Torez, and Lisitchansk areas. Data from these wells were published by Sachsenhofer et al. (2002). In this study, additional data (vitrinite reflectance and lithology) were obtained from boreholes located in the northern part of the basin, i.e., Kosiora, Osnovnaya, Gazeti Izvestiya, Tchesnokova, Olkhovatsky Site, Illytcha, Proletarskaya, Centr. Belyanka, and Zamkovskaya mines. The objectives of this article are to (1) reconstruct the burial and thermal history of the DF; (2) evaluate the factors controlling the coalification pattern; (3) model the processes of hydrocarbon generation, expulsion, migration, accumulation, and loss; (4) estimate the amount of methane trapped in the study part of the DF; and (5) predict the main zones of methane accumulation.

REGIONAL GEOLOGIC SETTING

The Dniepr-Donets depression (DDD) is a large Late Devonian Pripyat-Dniepr-Donets-Karpinsky rift system located at the southern part of the East European craton (Figure 1). Prior to the rift, the region was a platform in which Middle Devonian and lower Frasnian sediments were deposited (Alekseev et al., 1996; Stovba et al., 1996). A major postrift subsidence occurred during the Carboniferous and Lower Permian (Sakmarian) under the sediment load (Stovba et al., 1996; Van Wees et al., 1996; Sachsenhofer et al., 2002) or a tectonic reactivation (Izart et al., 2003a). The Donbas Foldbelt is generally considered to have been profoundly uplifted at the end of the Early Permian in response to the build-up of stresses emanating from the Hercynian Caucasus–Uralian orogens (Milanovsky, 1992). Compression resulted in a thrusting, folding, and inversion movement particularly intense southeastward of the DDB (Popov, 1966; Belokon, 1971; Pogrebnov, 1971; Mikhalyev, 1976; Nagorny and Nagorny, 1976; Privalov, 1998). The following uplift and erosion of the Permian successions are reflected by a basinwide unconformity (Nagorny and Nagorny, 1976; Privalov et al. 1998; Sachsenhofer et al., 2002; Spiegel et al., 2004). The Triassic–Tertiary postrift platform sequence is characterized by unconformity-bounded depositional sequences in response to tectonic deformation, uplift, and subsequent erosion (Kabyshev et al., 1998; Sachsenhofer et al., 2003; Spiegel et al., 2004). Seismic data led other authors to suggest that the strong compressional event (basin inversion) occurred during the Late Cretaceous–early Tertiary because of Cimmerian and Alpine orogenies (Stovba et al., 1996; Stovba and Stephenson, 1999; Saintot et al., 2003a, b; Stephenson et al., 2006). So, the structure of the southeastern part of the DDB is thought to be controlled by Early Permian and/or Late Cretaceous–early Tertiary inversion phases.

The DF is the deformed and structurally inverted part of the DDB (Figure 1) dominated by west-northwest–east-southeast–striking anticlines and synclines. The main anticline, the largest fold in this area, is bordered by two gentle synclines: main and south synclines (Figure 1). The thickness and lithology of the Devonian rift sediments still remain unknown because these deeply buried strata have not been drilled yet. Mesozoic and Cenozoic strata are absent in the study area (Figure 1). The

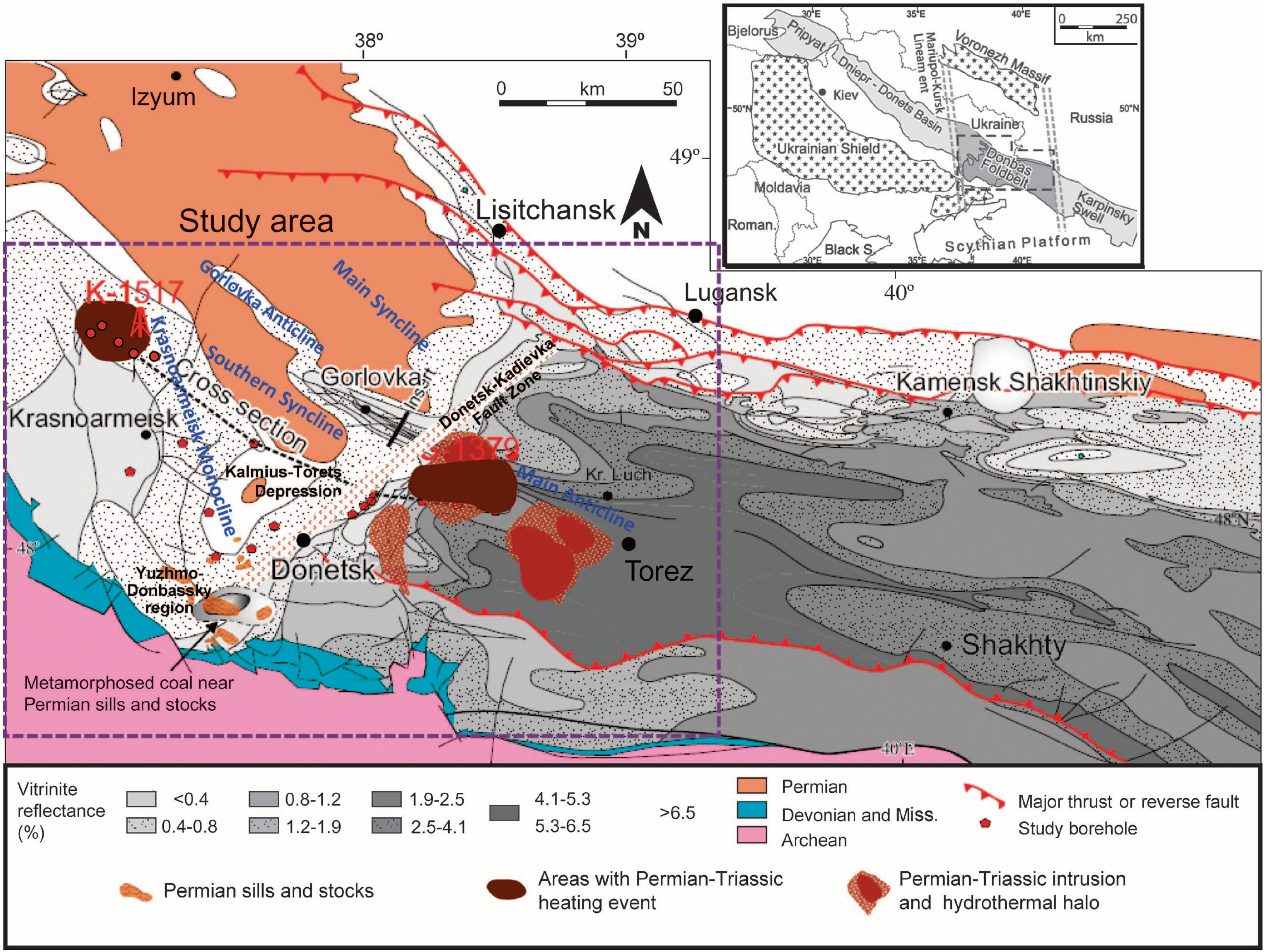

Figure 1. Location of the study area in the Donbas fold belt in the southeast of Ukraine and the map of vitrinite reflectance at the top of the Carboniferous section (modified from Levenshtein et al., 1991).

youngest Paleozoic succession is up to 15.3 km (9.5 mi) thick with Lower Permian and Carboniferous strata as preserved (Figure 2). The latter alone can reach up to 13.3 km (8.2 mi) and consists of cyclic successions of marine, continental, and lagoonal facies (Izart et al., 2003a, b, 2006; Sachsenhofer et al., 2003). Tournaisian–lower Visean strata are mainly composed of marine limestones. The overlying upper Visean–Gzelian strata consist of clastic rocks, mainly shales, interbedded with limestone and coal beds (Figure 2). The overlying upper Visean–Gzelian strata consist of clastic rocks, mainly shales, interbedded with limestone and coal beds (Figure 2). The Carboniferous sequence is divided into early (C1), middle (C2), and late (C3). Based on fauna analyses of major marine limestone horizons, these are further subdivided into units called suites according to local nomenclature and designated by capital letters (Aizenverg et al., 1975). From bottom to top, C1 is composed of suites A–D, C2 comprises suites E–M, and C3 contains suites N–P. Finally, sandstones, limestones, and evaporites (salt or anhydrite) were deposited during the Asselian–Sakmarian (Early Permian). Carboniferous succession alone is preserved toward the southeastern part of the study area. However, up to 2.2 km (1.3 mi) of Lower Permian rocks are present in the main and south synclines (Figure 2). Extensive postrift magmatic events have been reported in the DF. Permian sills and stocks with alkaline rocks occur southwest of Donetsk. Permian–Triassic magmatic events (andesitic magmatism) occurred in the south syncline (southeast of Gorlovka) and in the northern Krasnoarmeisk monocline (Aleksandrov et al., 1996; Sachsenhofer et al., 2002; Spiegel et al., 2004). Figure 2 also shows that magmatic events occurred during the Triassic and Jurassic (Lazarenko et al., 1975, de Boorder et al., 1996, Privalov, 2000, Alexandre et al., 2004).

PETROLEUM SYSTEM

Nobody had prognosticated the presence of oil and gas in the DDB before 1931; the assumption that Donbas was a coal-bearing basin dominated at that time. Based on the prognosis of N. S. Shatsky in 1931, the initial oil and gas exploration phase was in 1936–1937 under the leadership of F. O. Lysenko in 1932–1936. An excellent review of the history of the oil and gas exploration in the DDB can be found in the articles of Kabyshev et al. (1998) and Ulmishek (2001). One can date the beginning of the oil and gas exploration in the DF at 1950 with the discovery of the gigantic gas-condensate Shebelinka deposit. Indeed, recent investigations show that this giant gas field is almost located within the DF (Privalov et al., 2007). In 1958, massive hydrocarbon prospecting resulted in the discovery of some 15 commercial gas deposits along the northern marginal fault of the DF. In the 1990s, U.S. Geological Survey studies identified the presence of coalbed methane accumulations in the DF (Law et al., 1998).

The main oil- and gas-generating source rocks identified in the DDB are Pennsylvanian marine shales and carbonates (Kabyshev et al., 1998; Ulmishek, 2001). Shales and carbonates in the Devonian strata are suspected to be potential source rocks, as well as Pennsylvanian and Mississippian shales. The function of Carboniferous coal seams as a source rock for gas and oil is still uncertain (Ulmishek, 2001). However, vitrinite reflectance values suggest that the Carboniferous coals could have generated gas in the eastern half and oil in the western half of the study area (Figure 1). Works of Sachsenhofer et al. (2003) and Alsaab et al. (2007) have shown that Carboniferous coals from the DF can be regarded as effective gas- and oil-prone source rocks.

Hydrocarbon accumulations are trapped in structural (anticlinal, synclinal, and fault block) and stratigraphic (reef sand pinch-out) traps at depths of up to 6200 m (20,341 ft) in the DDB (Ulmishek et al., 1994; Kabyshev et al., 1998; Vakarchuk et al., 2006; Privalov et al., 2007). Deeply buried carbonates and clastic rocks of Pennsylvanian and Devonian age could have poor reservoir properties because of high temperature and overpressure. Mississippian and Lower Permian clastics and, to a much lesser degree, the carbonates are the reservoir rocks. Carboniferous coal seams can also be potential reservoir rocks for oil and gas (Levine, 1993). Figure 2 shows that the Carboniferous coal-bearing reservoir

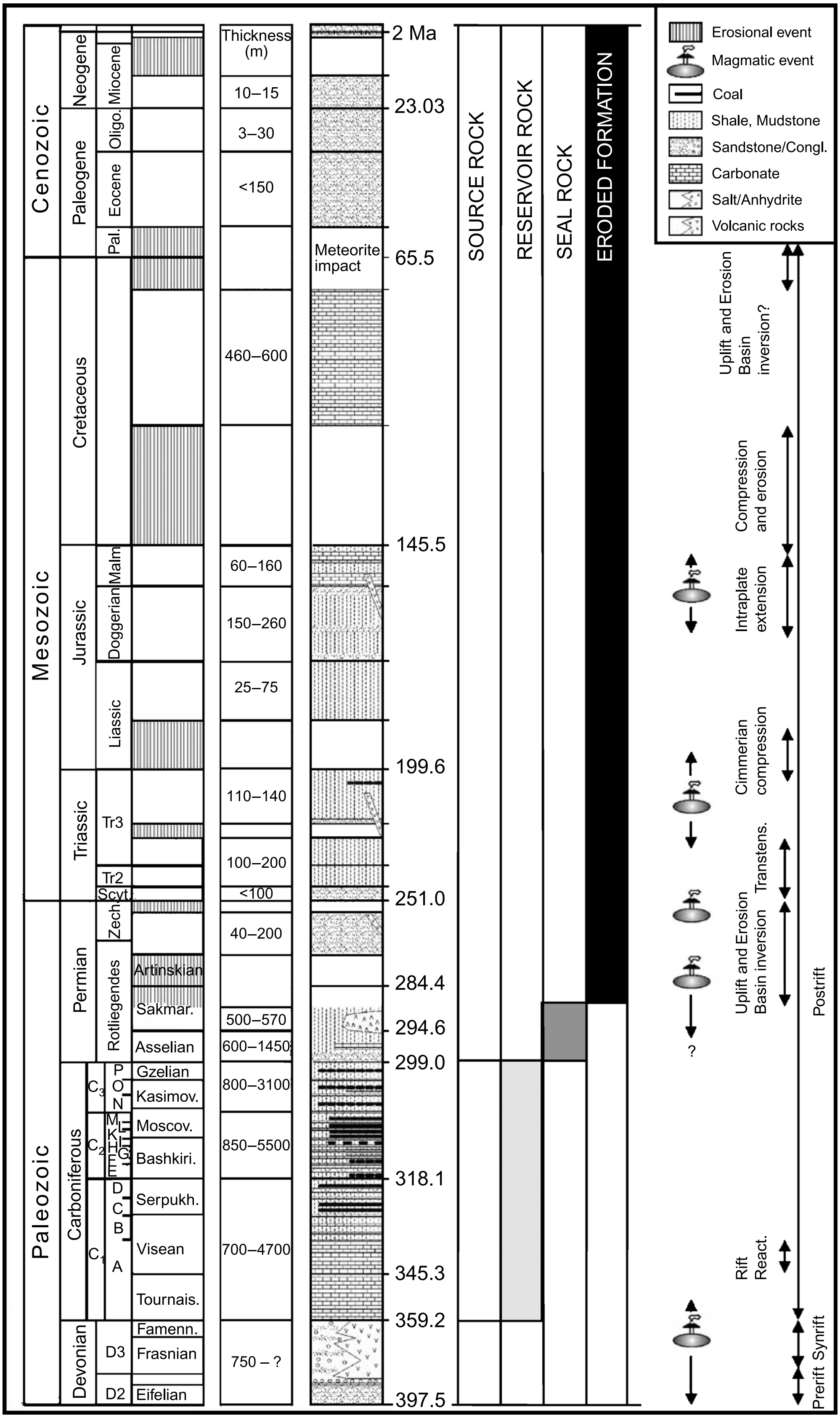

Figure 2. Chrono- and lithostratigraphy of the Donbas fold belt showing the distribution of source rocks, potential reservoirs, sealing beds, and eroded formations in the study area. Major magmatic and tectonic events are also shown.

rocks are sealed by Lower Permian salt-bearing sequences.

Hydrocarbon trapping mechanisms are different between the non- and inverted parts of the DDB. Main hydrocarbon accumulations are located in the non- and mildly inverted parts of the DDB, suggesting that inversion movements caused the loss of hydrocarbons to the surface and the modification of trap geometries, as well as the development of secondary traps that can be charged with hydrocarbons escaping from pre-existing primary traps (Kabyshev et al., 1998). However, conventional gas deposits are known on the north of the Kalmius-Torets depression where Early Permian salt-bearing sequences have been preserved (Privalov et al., 2007). So, the almost unexplored northeastern margin of the study area, where reservoir rocks are capped by a Lower Permian salt seal, may be a viable commercial prospect (Figure 1). In the southeastern flank of the study area, all strata younger than the Carboniferous sections were completely removed by several erosional phases occurring during the basin evolution (Figure 1). However, the Carboniferous coal-bearing strata can be potential coalbed-thermogenic methane resources whose amounts mainly depend on the rank and presence of endogenic CO_2 (Privalov et al., 2004b; Privalov et al., 2007). Viable prospective sites of coalbed methane trapped within fractured and sealed secondary reservoirs are suspected between the Donetsk and Torez regions (Privalov et al., 2007).

METHODS

Physical Rock Properties

Detailed information on the thickness and lithological composition was provided by the Donetsk State Regional Geological Survey and has been published for most wells by Sachsenhofer et al. (2002). Average lithological compositions of Carboniferous suites in the Krasnoarmeisk and Kalmius-Torets regions and in the south and main synclines used for simulation are from Sachsenhofer et al. (2002). The simulation was also performed using the thermal conductivity, density, heat capacity,

Table 1. Lithological Composition of Carboniferous Suites in New Mines in the Northern Part of the Donets Fold Belt

Suite	Sandstone (%)	Siltstone (%)	Mudstone (%)	Coal (%)	Limestone (%)
Olkhovatsky Mine					
M	35.7	49.3	10.3	2.1	2.6
L	41	42.2	11.7	3.1	2
K	39	46	11.8	1.7	1.5
I	31	49.5	17.3	1.1	1.1
H	48.9	33.9	16	0.8	0.4
G	26.2	54.3	18.5	0.6	0.4
F	18	20	60	0.1	1.9
Kosiora Mine					
N	18	63.6	14.3	0.9	3.2
M	46	37	8.4	1.3	7.3
L	36.4	32.8	26.7	2	2.1
K	29.2	53.1	14.6	1.4	1.7
Menzhynsky Mine					
D	17	40	40	1	2
C	25	35.5	35.5	3	1
B	17	40.5	40.5	1	1
M	21	36.5	36.5	1	5
L	27	33.5	33.5	2.5	3.5
K	39	28	28	1.4	3.6
Gazeti Izvestiya Mine					
L	50	23.5	23.5	1.7	1.3
K	22	36.2	36.2	2.7	2.9
Tchesnokova Mine					
N	26.4	38	34.3	0.04	1.26
M	29.6	42	14	1.4	13
L	36	34.3	22.8	2.5	4.4
K	39	41	15	1.4	3.6
Illytcha Mine					
N	24.4	39.6	31.5	0.7	3.8
M	29.6	51	5	1.4	13
L	36	37.1	18.7	3.5	4.7
K	33	38.3	21.3	2.9	4.5
Proletarskaya Mine					
M	23	35.4	20	3.6	18
L	39	31.4	12	8.6	9
K	53	20.3	17	2.7	7
Zamkovskaya Mine					
L	21	52	18	4	5
K	32	48	12	3	5
I	28	53	16	2	6
H	35	55	7	1	2
G	56	24	17	1	2

Table 2. New Vitrinite Reflectance (R_o) Data Observed in Coal Mines in Donbas*

Kosiora Mine					Centr. Belyanka Mine		
Well	Б4534		Б4659		Well	M686	
	Depth	R_o (%)	Depth	R_o (%)		Depth	R_o (%)
	646.24	2.49	691.42	2.57		695	1.02
	948.14	2.82	968.32	2.78		971	1.12
	1085.49	2.66	1140.72	2.72		1051	1.25
	1334.89	3.25	1382.47	3.25		1195	1.53
			1846.15	3.34		1405	1.59
						1545	1.62

Olkhovatskaya Mine								
Well	Ц-1294		Ц-1259		Ц-1248		Ц-1202	
	Depth	R_o (%)	Depth	R_o (%)	Depth	R_o (%)	Depth	R_o (%)
	464	2.6	765	3.02	761	3.74	775	3.79
	1072	2.97	1188	3.09	1102	3.96	819	4.11
	1556	4.3	1324	3.77	1158	4.1	1079	4.21
					1449	4.32	1140	4.4

Zamkovskaya Mine					Proletarskaya Mine		
Well	Б2234		1490		Well	2770	
	Depth	R_o (%)	Depth	R_o (%)		Depth	R_o (%)
	1294.93	1.87	984.9	1.92		344.75	0.52
	1365.52	1.88	1129.8	1.95		441.75	0.56
	1483.72	2.04	1256.8	1.97		539.75	0.59
						645.32	0.64
						820.32	0.7

Illytcha Mine					Tchesnokova Mine				
Well	Б0632		Б3292		Well	1781		3300	
	Depth	R_o (%)	Depth	R_o (%)		Depth	R_o (%)	Depth	R_o (%)
	628	0.92	525	0.95		514.8	0.87	575.2	0.9
	711	0.94	582	0.96		644.8	0.95	702.2	0.95
	762	0.95	588	1.05		775.8	0.99	766.04	1.07
	801	0.96	647	1.09		965.8	1.02	870.28	1.08
	876	1.06	683	1.1		994.8	1.07	1151.28	1.22
	1000	1.2	936	1.2				1240.28	1.37
	1102	1.22	1016.3	1.22					
	1132	1.26	1041.3	1.29					

Table 2. Continued

	Osnovnaya Mine					
Well	У-3971		У-4033		У-4059	
	Depth	R_o (%)	Depth	R_o (%)	Depth	R_o (%)
	770.1	3.27	798.8	4.28	694.98	3.28
	813.4	3.98	837.36	4.38	737.04	3.8
	912.08	4.3	964	4.5	832.1	4.3

*See Figure 1 for the location of the mines. Depths are in meters.

and permeability data given by Sachsenhofer et al. (2002). The average lithological composition of Carboniferous suites in the northern part of the DF is given in Table 1. The dimensions, depth, and thermal and physical properties of andesitic intrusions in the western and eastern parts have also been published by Sachsenhofer et al. (2002).

Coal Beds

Random vitrinite reflectance (R_o) data of 248 coal samples were published by Sachsenhofer et al. (2002) and are used in the present article. Additional vitrinite reflectance data were measured in the coal mines in the northern part of the DF (Table 2). The coal is generally of anthracite rank in the central part of the DF. Subbituminous and bituminous coals are restricted to the western and northern basin margins (Figure 1). This rank pattern was controlled by a Carboniferous–Early Permian subsidence. This pattern was distorted and overprinted in some areas because of thermal events associated with the Permian–Triassic magmatic pulses (Sachsenhofer et al., 2002; Privalov et al., 2004a). The Carboniferous section hosts more than 300 coal seams. About 130 coal seams are thicker than 0.45 m (1.4 ft). Coal seams are typically thin (<1 m) but have a wide lateral extent. The total coal thickness is about 60 m (197 ft) (Sachsenhofer et al., 2003; Privalov et al., 2004a). Seams in the Serpukhovian (upper Mississippian; suites C and D) and Moscovian (middle Pennsylvanian; suites K–M) sections (Figure 2) are the most important. Table 3 gives the TOC (%) and HI (mg HC/g TOC) values of the coals collected in suites B–O. The TOC values of Carboniferous suites were calculated by considering the percentages of the coal reported in Table 1.

Heat Flow and Erosion Histories

The impacts of Permian–Triassic magmatic intrusions are taken into account by an increase in HF values (Allen and Allen, 1990). Fission-track data and basin modeling indicate that the andesitic magmatism was a very important factor in determining the high maturity of coal beds in the DF (Sachsenhofer et al., 2002; Spiegel et al., 2004). However, with the exception of contact metamorphism, Permian magmatic sills and stocks southwest of Donetsk did not significantly change the regional HF and, therefore, the coalification pattern because the volume of the magma was not high enough (Privalov

Table 3. Total Organic Content (TOC) and Hydrogen Index (HI) Data Used for the Modeling Study in the Donets Basin*

Suites	TOC (wt. %)	HI (mg HC/g TOC)
O	52	210
N	78	306
M	89	298
L	75	264
K	84	282
I	83	276
H	86	310
G	64	290
F	69	279
E	76	257
D	84	249
C	81	260
B	62	218

*See Table 1 for the percent of coal in the Carboniferous suites.

et al., 1998). The HF history of the DF proposed by Sachsenhofer et al. (2002) using a basin modeling approach is as follows: (1) HF during maximum Permian burial was in the range of 40–75 mW/m^2, and (2) high HF values occurred after the maximum burial along the south syncline (up to 200 mW/m^2) and in the northern Krasnoarmeisk monocline (up to 150 mW/m^2), probably related to Permian–Triassic magmatic events.

Combining fission-track analysis and numerical modeling techniques, Spiegel et al. (2004) and Sachsenhofer et al. (2002) estimated the erosion during the Permian of approximately 2–3 km (1.2–1.8 mi) of sediment in the Krasnoarmeisk monocline and Kalmius-Torets depression and of approximately 4–6 km (2–4 mi) of sediment in the area east of the Donetsk-Kadievka fault zone. Low vitrinite reflectance values in the range of 0.6–0.7% (Sachsenhofer et al., 2003) indicate that less erosion occurred in the Yuzhno-Donbassky region. These results are in agreement with those of Nagorny and Nagorny (1976), which showed an erosion of about 15 km (9 mi) of sediment along the southern margin, 11 km (7 mi) in the center, and 2 km (1.2 mi) along the northern margin of the basin. From seismic reflection profiles along the northwestern margin of the DF, Stovba and Stephenson (1999) suggested that rocks up to 10 km (6 mi) thick were eroded.

Geological Models

Models for six cross sections (S1–S6; Figure 3a) were established for the study area and calibrated using vitrinite reflectance data. The input data include the thickness of the stratigraphic suites, physical properties of rocks, HF, temperature at the sediment-water interface, paleowater depth, and structural data. Figure 3b shows the north-northwest–south-southeast–trending cross section S1 together with the location of the wells. Figure 3b also shows that the Carboniferous suites are affected by faults and associated folds in the central and southeastern parts and by two magmatic intrusions of andesitic type (Sachsenhofer et al., 2002; Spiegel et al., 2004). Cross sections S2, S3, S4, S5, and S6 (Figure 3a) run parallel to the Donbas Basin deep seismic refraction experiments and Donbas Basin deep seismic reflection experiments (DOBRE) refraction and reflection seismic line (Grad et al., 2003; Maystrenko et al., 2003). All cross sections were imported and digitized in PetroBuilder 2-D.

Basin Modeling and Map Construction

PetroMod software was used to reconstruct the burial and thermal history of the DF and to model hydrocarbon generation, migration, and trapping. Using stratigraphic, structural, petrophysical, and organic geochemical data, six 2-D numerical models were developed for the study area of the DF. The structural models are based on six regional cross sections constructed from the geological map of the basin and the DOBRE seismic line. The simulation of the thermal history relies on understanding the thermal properties of different formations, HF history, thickness of eroded sediment, and present-day subsurface temperature. The simulation began by defining vertical grid lines and horizontal event lines in each cross section. For each cell, input data, i.e., thickness, age at upper and lower boundary, lithological properties, and HF, were defined and entered (Poelchau et al., 1997; Lutz et al., 2004). Furthermore, total organic carbon contents and HI values were used for the calculation of hydrocarbon generation from Carboniferous suites (Büker et al., 1995; Poelchau et al., 1997). Because of high ranks of Carboniferous Donets coals in most parts of the study area in the DF, Burnham's (1989) kinetic model of methane generation from coal has been selected for the numerical simulation in this work.

Numerical 1-D and 2-D models were calibrated by modifying the HF and the thickness of eroded rocks until a satisfactory fit between measured and simulated vitrinite reflectance values was reached. Basically, vitrinite reflectance is simulated using the kinetic EASY%R_o algorithm (Sweeney and Burnham, 1990). However, this algorithm is only applicable for R_o maturation values as high as 4.69%. Vitrinite reflectance values higher than 6% are observed in the DF. Consequently, an extended model (extended EASY%R_o model), depicted in Figure 4, was used for the calibration of thermal models up to 6.23% (Everlien, 1996). Note that,

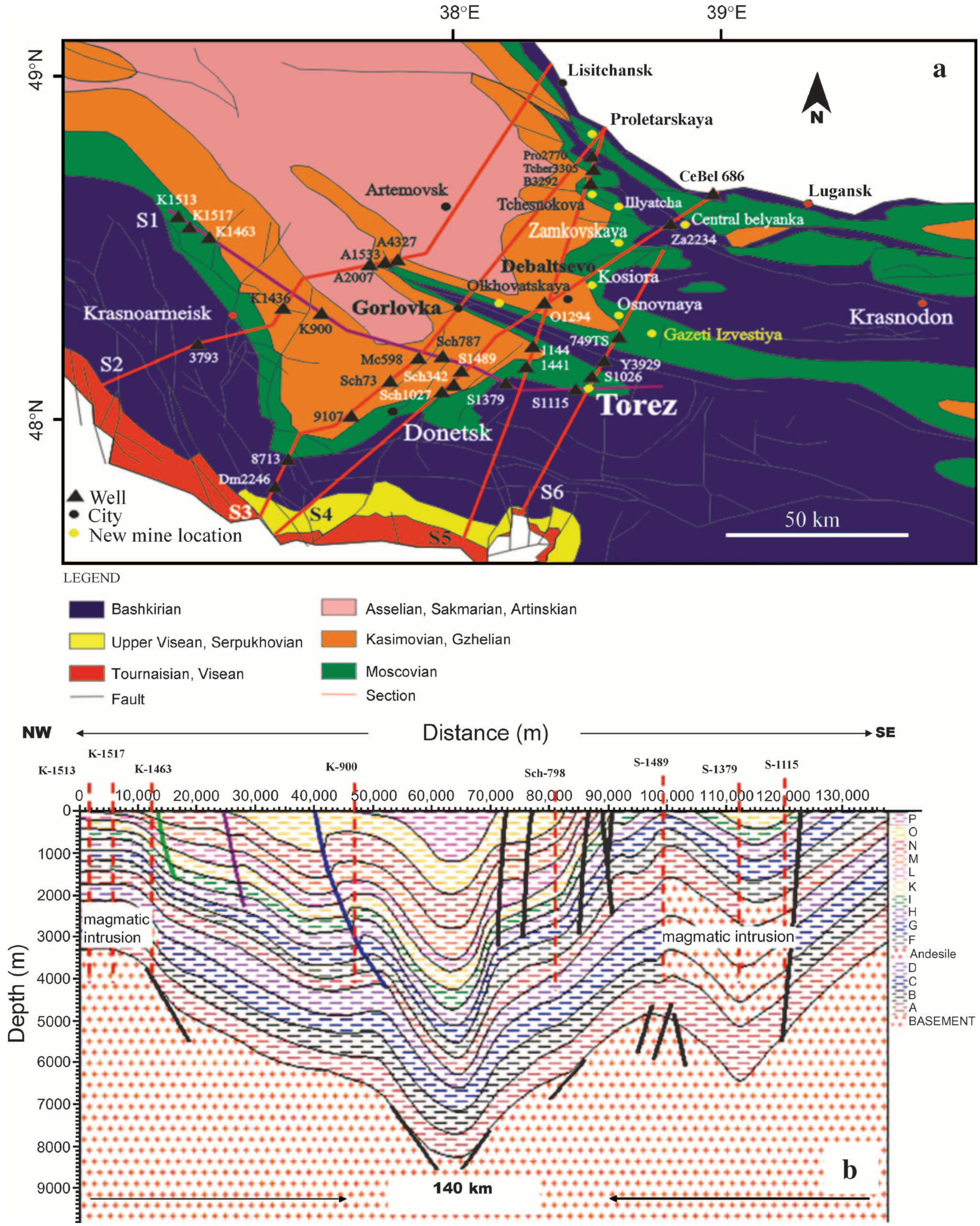

Figure 3. (a) Geological map of the Donbas fold belt showing the Permian–Carboniferous stages, and the cross sections (S1, S2, S3, S4, S5, and S6), new mines, and wells used in this article. (b) Cross section S1 showing faults, key wells (vertical dashed red lines), Devonian basement, Carboniferous suites (A–O), Permian seal rocks (P), and magmatic intrusions.

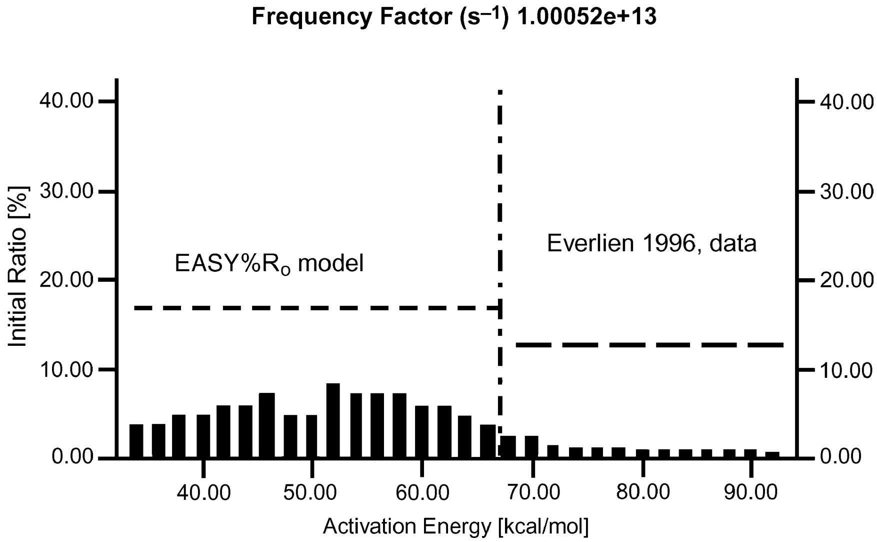

Figure 4. Activation energy distribution for the extended EASY%R_o model integrated in PetroMod software.

up to 4.6% R_o, the models yield identical results as shown in Figure 4.

The 2-D basin modeling of cross section S1 is depicted in Figure 5. By using kriging algorithms in Surfer software, isoline maps were built at a depth of 500 m (1640 ft) for vitrinite reflectance, erosion, methane generation, and accumulation in the DF.

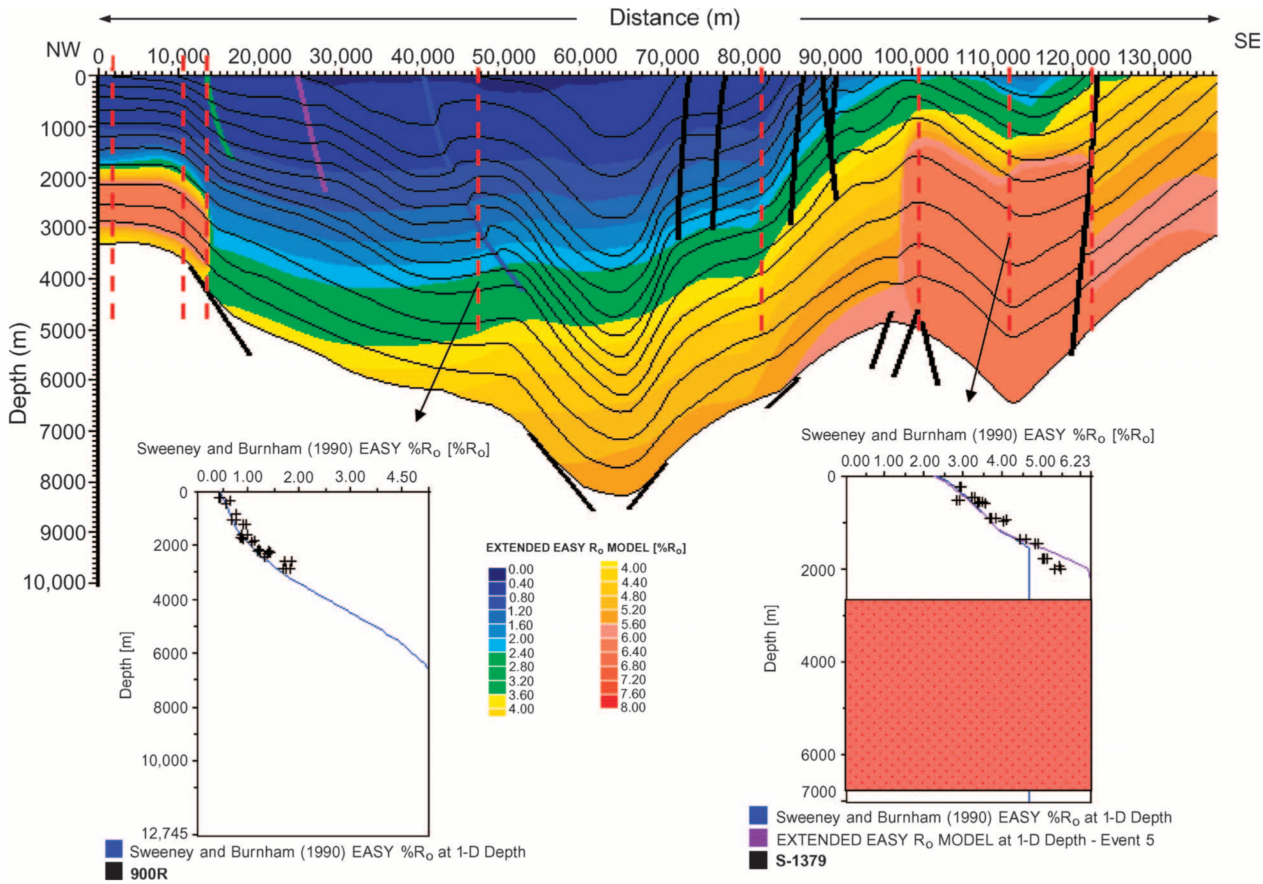

Figure 5. The 2-D basin modeling derived from calibration curves between measured and calculated vitrinite reflectance (% R_o) values for cross section S1.

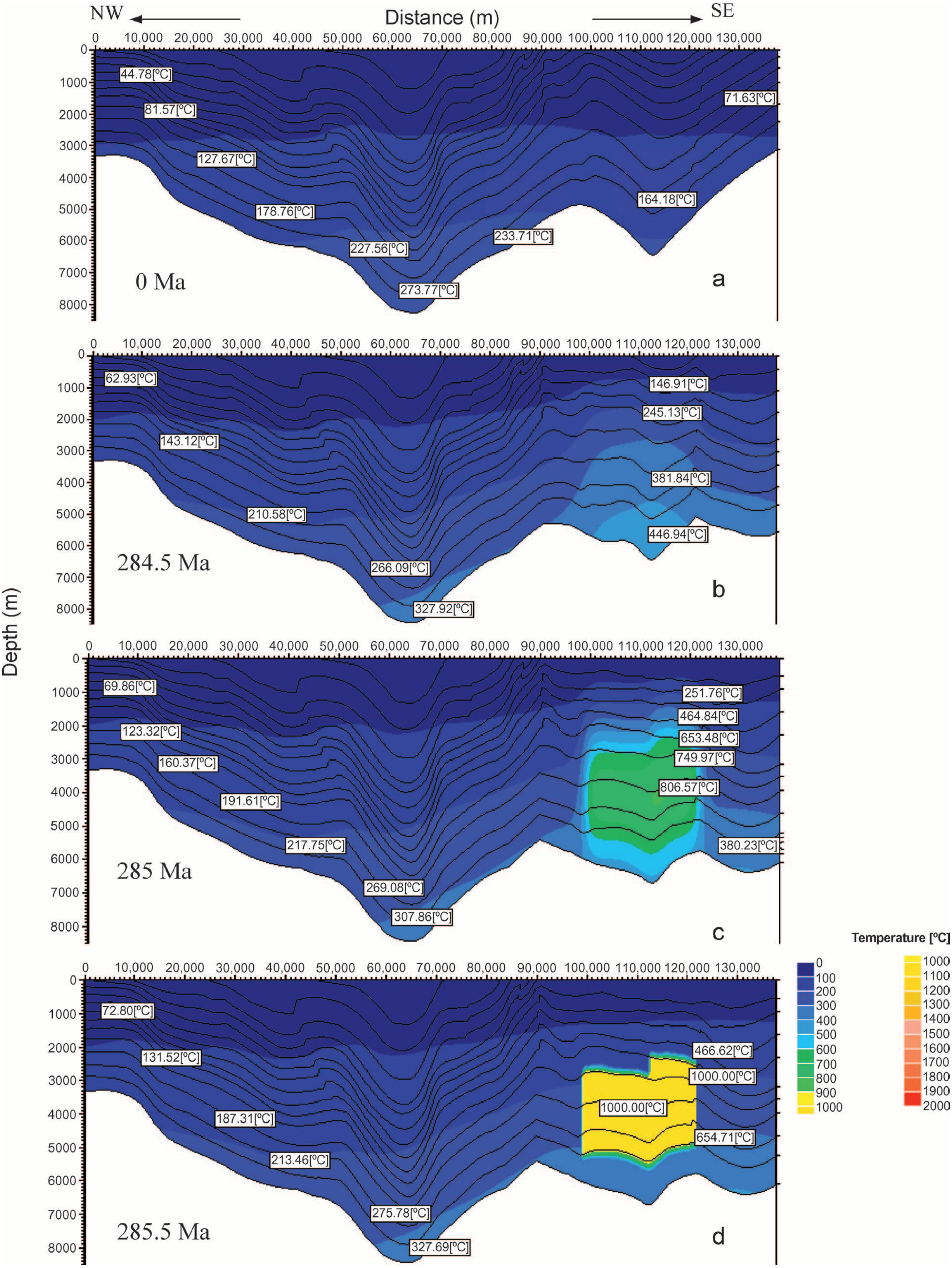

Figure 6. Simulated Permian and present-day temperature profiles along cross section S1. Note that the paleoisotherms become shallow in the eastern part of the cross section during magmatic intrusion.

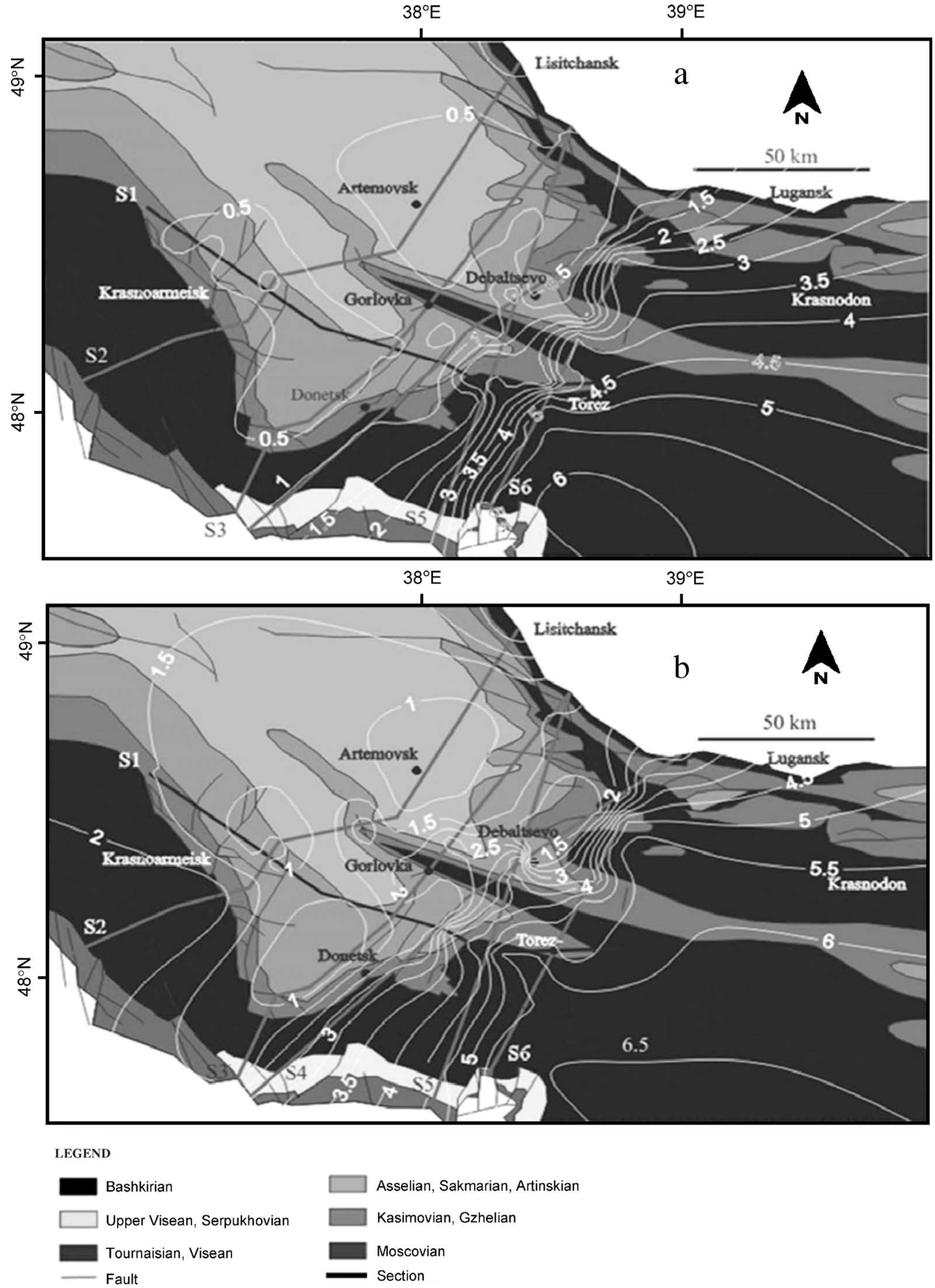

Figure 7. Simulated maps of coal rank based on 2-D modeling: (a) surface and (b) depth of 2000 m (6562 ft).

BURIAL AND THERMAL HISTORY

Only the scenario based on a major Late Permian uplift was considered in the present study (Sachsenhofer et al., 2002). Devonian synrift formations are not taken into account in this study, as well as pre-Carboniferous subsidence. The Carboniferous–Early Permian basin subsidence was followed by an uplift at the end of the Early Permian and a subsequent erosion of approximately 2100 m (6890 ft). Another erosional phase of approximately 300–400 m (984–1312 ft) occurred during the Late Cretaceous. The HF history for well Sch-1027 can be summarized as follows: (1) HF approximately

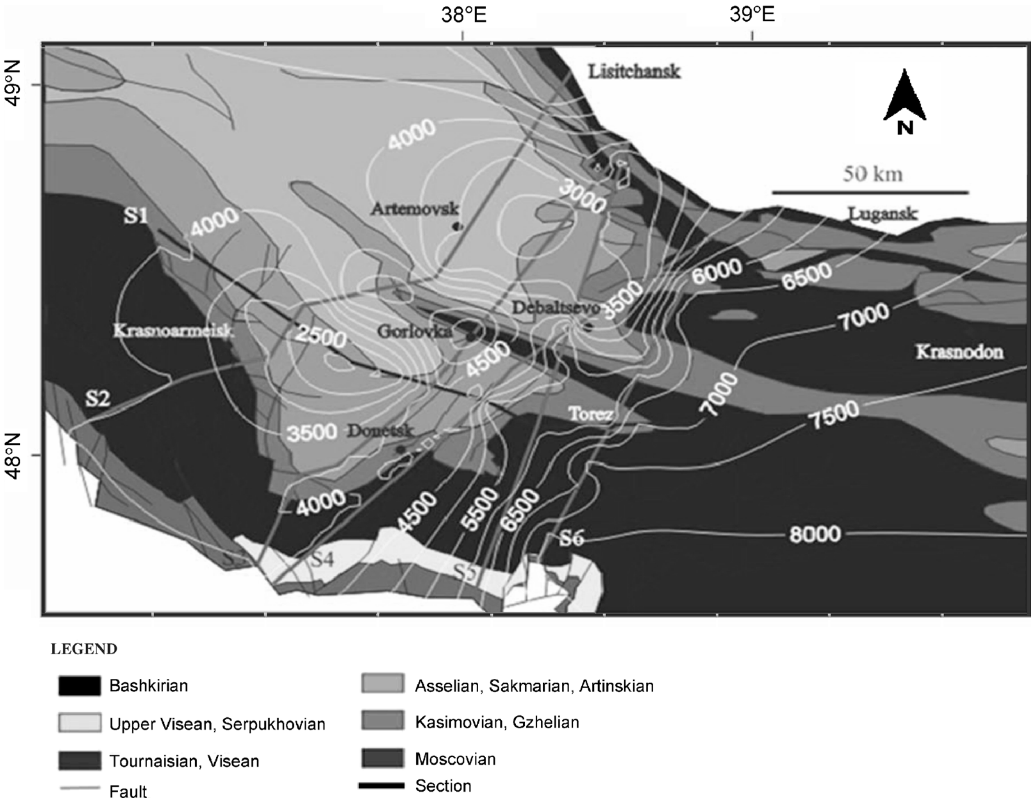

Figure 8. Total thickness of eroded sediment estimated using a 2-D modeling approach in the Donbas fold belt.

65 mW/m^2 during the Carboniferous–Early Permian subsidence, (2) HF approximately 150 mW/m^2 in the south syncline related to Permian–Triassic magmatic events, and (3) HF approximately 57 mW/m^2 during Mesozoic and Cenozoic postrift phases.

The 2-D modeling enables a more precise description of the temperature distribution in sedimentary basins. Figure 6 shows the distribution of paleotemperatures and present-day temperatures for cross section S1. Paleoisotherms shallow toward the eastern part of the profile in the south syncline between 285.5 and 284.5 Ma (Figure 6) and in the north part of the Krasnoarmeisk region because of magmatic events. The magmatic intrusion occurred at a temperature of about 1000°C in the south syncline (Sachsenhofer et al., 2002). The temperature of the pluton apparently decreased from 1000 to 750°C over about 0.5 m.y. (between 285.5 and 285 Ma) and then to 400°C at 284.5 Ma (Figure 6). Temperatures of about 900°C are suspected during the magmatic event in the Krasnoarmeisk region. The HF values assumed at the base of the sedimentary sequence in the zones around plutons for which a good fit was obtained between measured and calculated vitrinite reflectance values are (1) 120 mW/m^2 for the Permian sills and stocks southwest of Donetsk and (2) 150 and 130 mW/m^2 for the Permian–Triassic andesitic magmatism in the south syncline and in the northern Krasnoarmeisk monocline, respectively. The distribution of the present-day temperature in Figure 6a shows subhorizontal isotherms with a maximum temperature of 300°C recorded in the center of the basin at a depth of 8 km (5 mi). Cross sections S2, S3, S4, S5, and S6 were also modeled and calibrated using vitrinite reflectance data from more than 40 wells.

The present-day coalification pattern is shown in this contribution as vitrinite reflectance maps reconstructed from 2-D modeling results on the six studied cross sections. Following Hilt's rule, vitrinite reflectance values increase with depth (Figure 7). For instance, vitrinite reflectance in

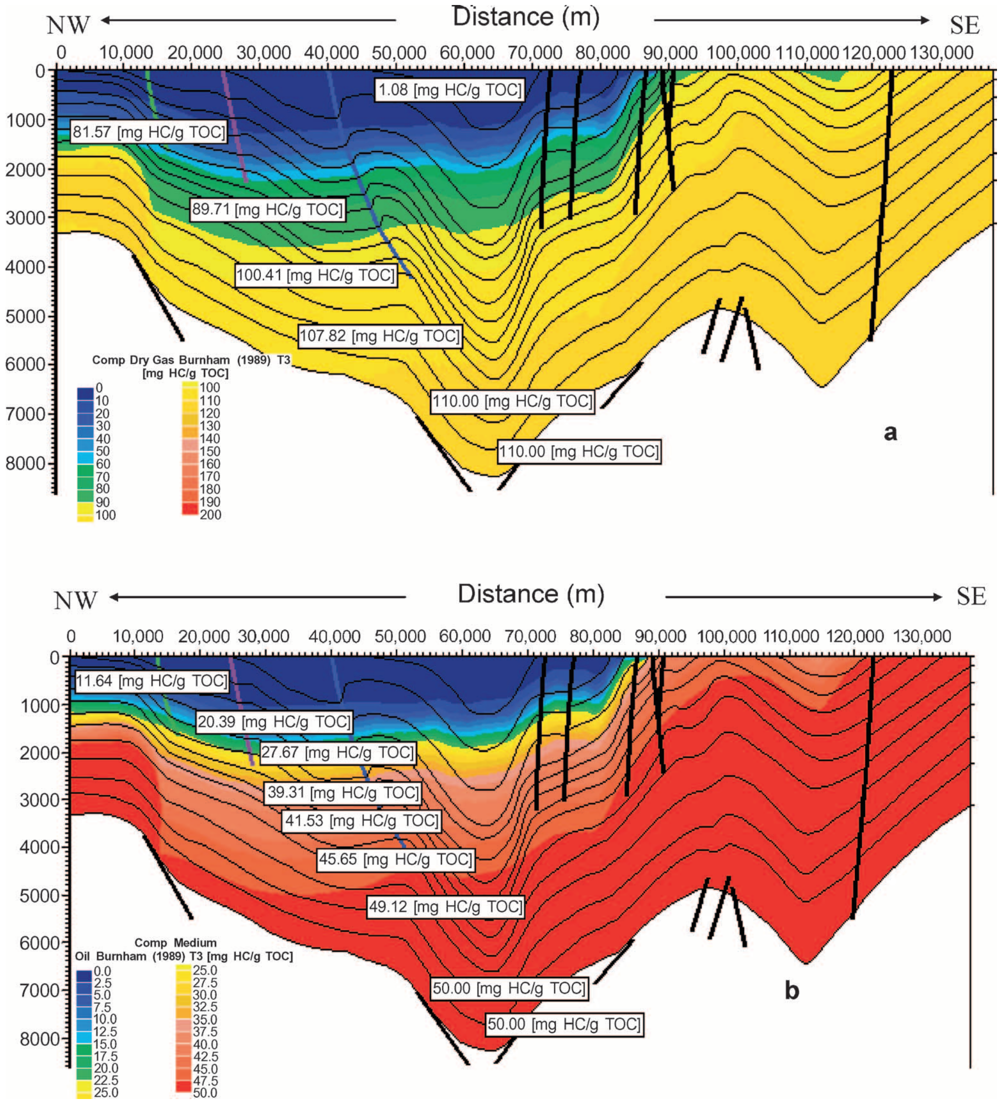

Figure 9. Theoretical generation potential for (a) gas and (b) oil in cross section S1. The Carboniferous suites buried at more than 4 km (2 mi) generated large amounts of methane (~110 mg/g TOC) and oil (~50 mg/g TOC). The shallow suites in the central and western areas have very low capacities for gas (~9 mg/g TOC) and oil (~78 mg/g TOC) generation.

the Krasnoarmeisk area is less than 0.5% at the surface and approximately 2% at a depth of 2000 m (6562 ft). In the southeast zone, near Torez, it is less than 4.5% at the surface and approximately 6–6.5% at a depth of 2000 m (6562 ft). Figure 7 also shows that the maturity level increases toward the eastern and southeastern parts of the DF. Vitrinite reflectance values indicate that coals are overmature in the southeastern half, although they are within the oil and gas window in the northwestern half of the study area. The difference across the study area can be related to the influence of Permian–Triassic HF events (Sachsenhofer et al., 2002).

Three erosional phases are suspected to occur after the compressional phases during the Late Permian, the Late Cretaceous, and the late Cenozoic in the Donets Basin. The Late Permian erosion is reported to be the most important, but, unfortunately, it was not possible to discriminate them because the two youngest strata are missing in the study area. Consequently, the total eroded thickness maps were constructed from 2-D modeling results in the six studied sections (Figure 8). The total erosion in the different parts of the DF is approximately 5 km (3 mi) near the main anticline, approximately 2–5 km (1.2–3 mi) in the main syncline with eroded thickness increasing toward the northeastern part to reach approximately 6.5 km (4 mi) near Lugansk, approximately 3–4 km (1.8–2 mi) northward near Lisitchansk, 2.5–4.5 km (1.5–2.7 mi) between Krasnoarmeisk and Donetsk, and approximately 5.5–6.5 km (3.4–4 mi) near Torez in the southeastern part of the

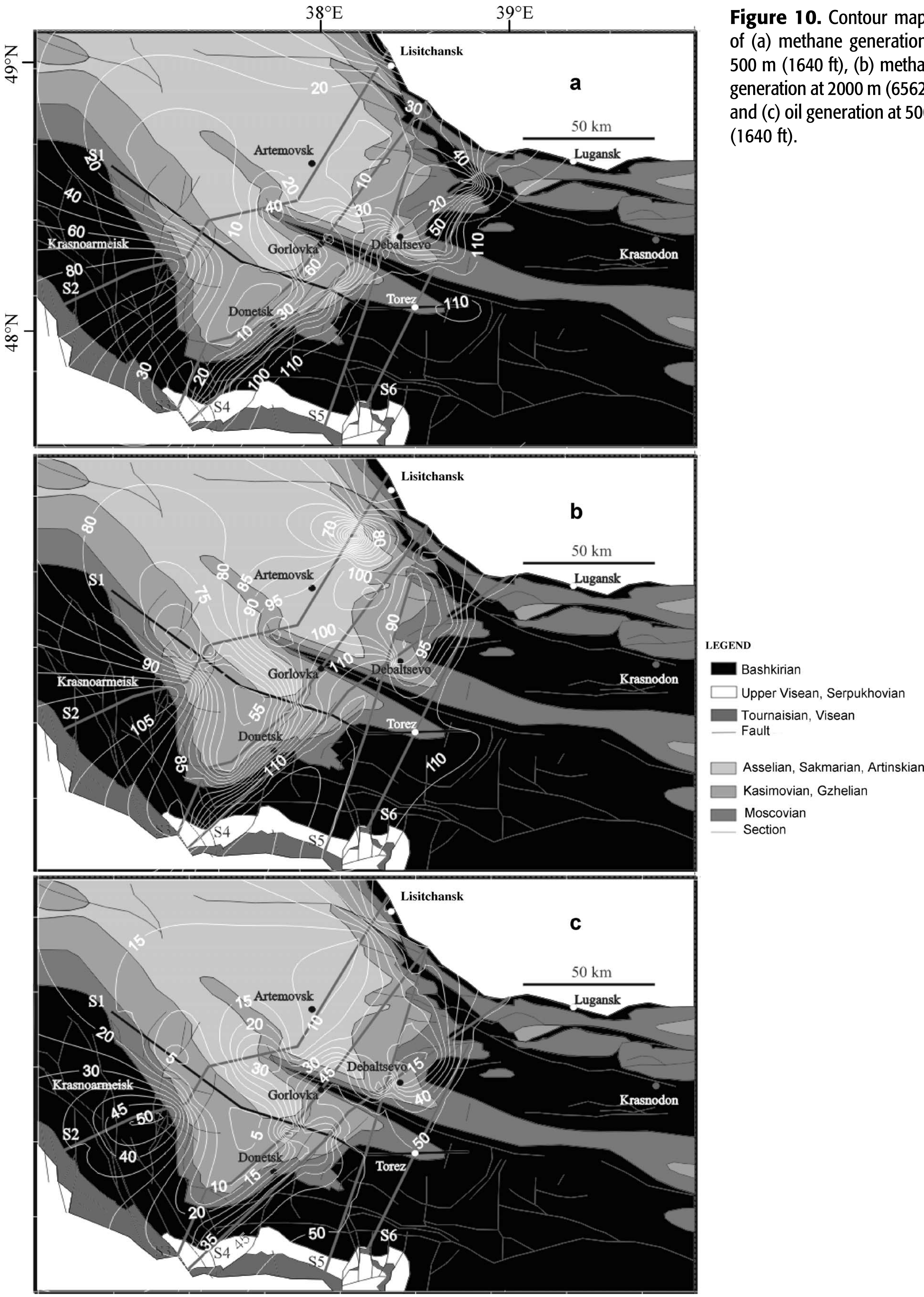

Figure 10. Contour maps of (a) methane generation at 500 m (1640 ft), (b) methane generation at 2000 m (6562 ft), and (c) oil generation at 500 m (1640 ft).

DF. Total erosion clearly increased strongly toward the eastern and southeastern parts of the study area, with maximal values reached in the zone of the south syncline at approximately 8 km (5 mi) (Figure 8). Figure 8 also shows a jump of the total erosion toward the eastern and southeastern parts, i.e., more rocks were eroded southeast of the Donetsk-Kadievka fault zone separating the two erosional domains (Sachsenhofer et al., 2002). However, the present study provides more details about the total erosion in the northern, northeastern, and northwestern parts of the DF (Figure 8). The distribution of the eroded section in the present study shows similar trends to those obtained by Nagorny and Nagorny (1976), Privalov et al. (1998, 2004a), and Spiegel et al. (2004).

PETROLEUM GENERATION

The source rocks considered in cross section S1 were suites B–O. Numerical simulation suggests that the Carboniferous–Early Permian subsidence induced a considerable transformation of kerogen into hydrocarbons. Contrasting trends are observed between the southeastern and northwestern parts of cross section S1 for suites B–K. The transformation ratio $(TR = 1200 \times (HI_0 - HI)/HI_0 \times (1200 - HI)$ with HI_0 as the initial petroleum potential) of kerogen is almost 100% in the southeastern part, whereas it is lower than 75% in the northwestern part near Krasnoarmeisk. Differences across S1 can be caused by the additional influence of Permian–Triassic magmatic events. The 2-D modeling of S1 shows that greater amounts of hydrocarbons, especially methane, were generated prior to basin inversion. As expected, source rocks fall into the gas-to-overmature zone in the southeastern part, whereas gas and oil are generated in the northwestern part. The theoretical potential of oil and gas generation along the cross section in Figure 9 shows that the Carboniferous suites buried at more than 4 km (2 mi) generated large amounts of methane (~110 mg/g TOC) and oil (~50 mg/g TOC). The shallow Carboniferous suites (L–O) in the central and western parts of S1 have very low capacities for gas (~9 mg/g TOC) and oil (~0.78 mg/g TOC) generation. As discussed previously, the amounts of gas and oil are lower in the northwestern part than in the southeastern part because of Permian–Triassic magmatic events. Hydrocarbon generation from Carboniferous coals was estimated on cross sections S2–S6 by the same method.

Maps of the generation of methane at 500 and 2000 m (1640 and 6562 ft) (Figure 10a, b) and oil at 500 m (1640 ft) (Figure 10c) were made using the 2-D modeling results. Figure 10a shows that the generation of methane at a depth of 500 m (1640 ft) was (1) low (10–30 mg CH_4/g TOC) in the northern part (main syncline), (2) moderate (40–80 mg CH_4/g TOC) in the western part (near Krasnoarmeisk), and (3) high (greater than 110 mg CH_4/g TOC) in the southeastern part of the study area. A comparison of Figure 10a and b reveals that the generation of methane increased with the burial and toward the southeastern part. Figure 10c shows similar trends of iso-oil generation lines with higher amounts (~60 mg/g TOC) in the eastern and southeastern parts of the study area. An increase in the rate of oil generation, likely caused by Permian–Triassic heating events, can be observed near Krasnoarmeisk (~50 mg/g TOC).

EXPULSION, MIGRATION, AND TRAPPING

Numerical 2-D modeling predicts three successive phases of oil expulsion in the DF during (1) the Mississippian and Early Permian for suites B and C in the northwestern part of the study area, for suites B–F in the central part, and for all in the southeastern part; (2) the Triassic and Jurassic mainly in the central part of S1; and (3) the Cretaceous mainly in the central part (Figure 11). Figure 11 also shows the effect of the magmatic events in the northwestern and southeastern parts of S1 on the occurrence of heating anomalies during the Permian–Triassic and of a major expulsion phase at the Late Permian. These three phases of oil expulsion from coals were also simulated for the other sections (S2, S3, S4, S5, and S6). Thus, these oil pulses along the DF indicate that the migration and the entrapment of hydrocarbons might occur in multiple stages.

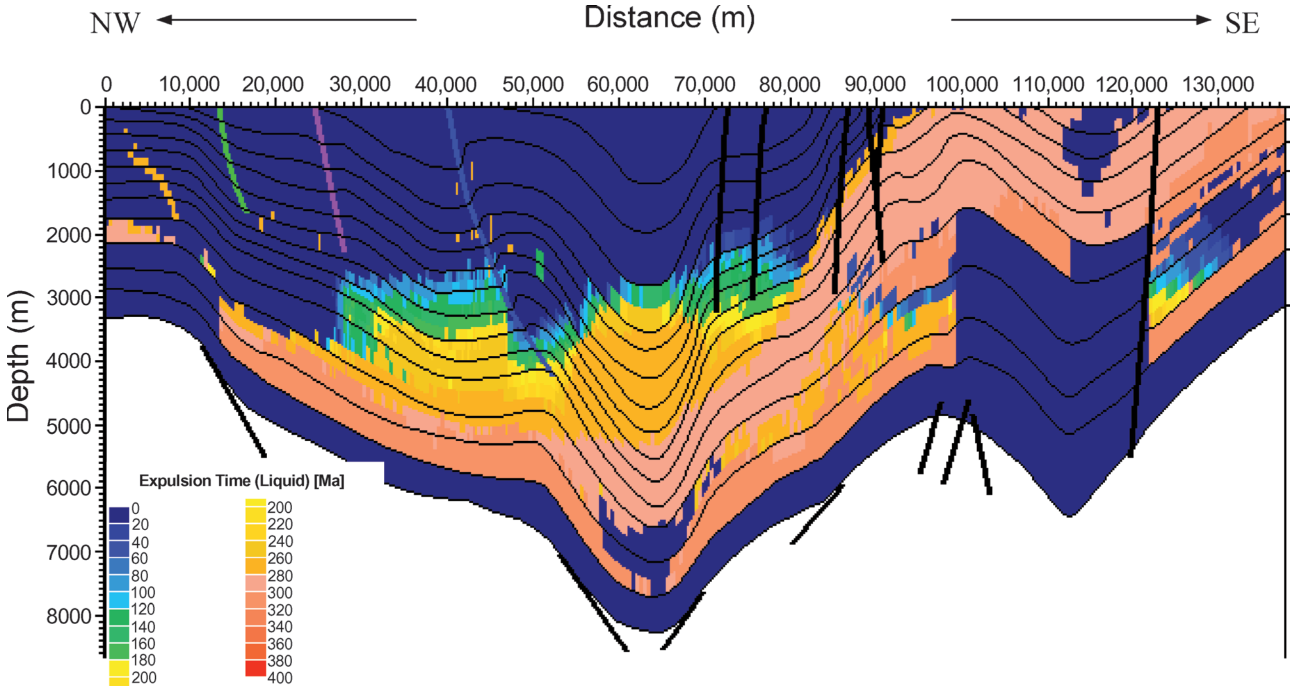

Figure 11. Model of oil expulsion in cross section S1.

Hydrocarbon migration was simulated along the six cross sections in the DF. Figure 12 shows the hydrocarbon saturation and the direction of oil and gas flow at different times along cross section S1. After the main phase of generation caused by the Carboniferous–Early Permian subsidence, hydrocarbons may have migrated not only laterally but also vertically through the fault system in the central and northwestern parts at the end of the Early Permian (Figure 12a). Hydrocarbon generation also occurred in the southeastern part of the basin because of the volcanism and high HF at this time. Hydrocarbons were generated and migrated during the Mesozoic (Figure 12b) and Cenozoic (Figure 12c) depositions. The generating amounts were much lower because (1) coals had already reached high maturity levels because of the Mississippian–Early Permian subsidence, and (2) the thicknesses of the Mesozoic and Cenozoic loads were not enough to induce a further maturation of coals. The existing traps may have been filled with migrating hydrocarbons. Basin inversion in the Early Permian and/or during the Late Cretaceous–early Tertiary caused the destruction of some primary accumulations and the migration of hydrocarbons either in newly formed secondary traps or to the surface (Kabyshev et al., 1998). Carboniferous rocks alone were preserved along cross section S1 because of uplifts and intense erosional processes at the Late Permian and Late Cretaceous–early Tertiary. The simulation predicts that hydrocarbon accumulations were destroyed and faults may have been a factor in the vertical migration and loss to the surface of hydrocarbons because of a lack of Lower Permian salt seals (Allan, 1989; Knipe, 1997).

IMPLICATION FOR EXPLORATION

The actual methane accumulation zones suspected in the DF were simulated by basin modeling. The present-day methane amounts accumulated in the Carboniferous coal-bearing strata were evaluated for cross sections S1, S2, and S6. Cross section S1 displays two methane accumulation zones that are close to the magmatic body with amounts in the range of 0.3–0.5 tcf of methane. Cross section S2 is the richest cross section in the methane reservoirs, especially in the south and main synclines with amounts from 0.2 to 2.0 tcf of methane. Cross section S6 is located in the anthracite zone of the DF. Three main methane accumulation zones are

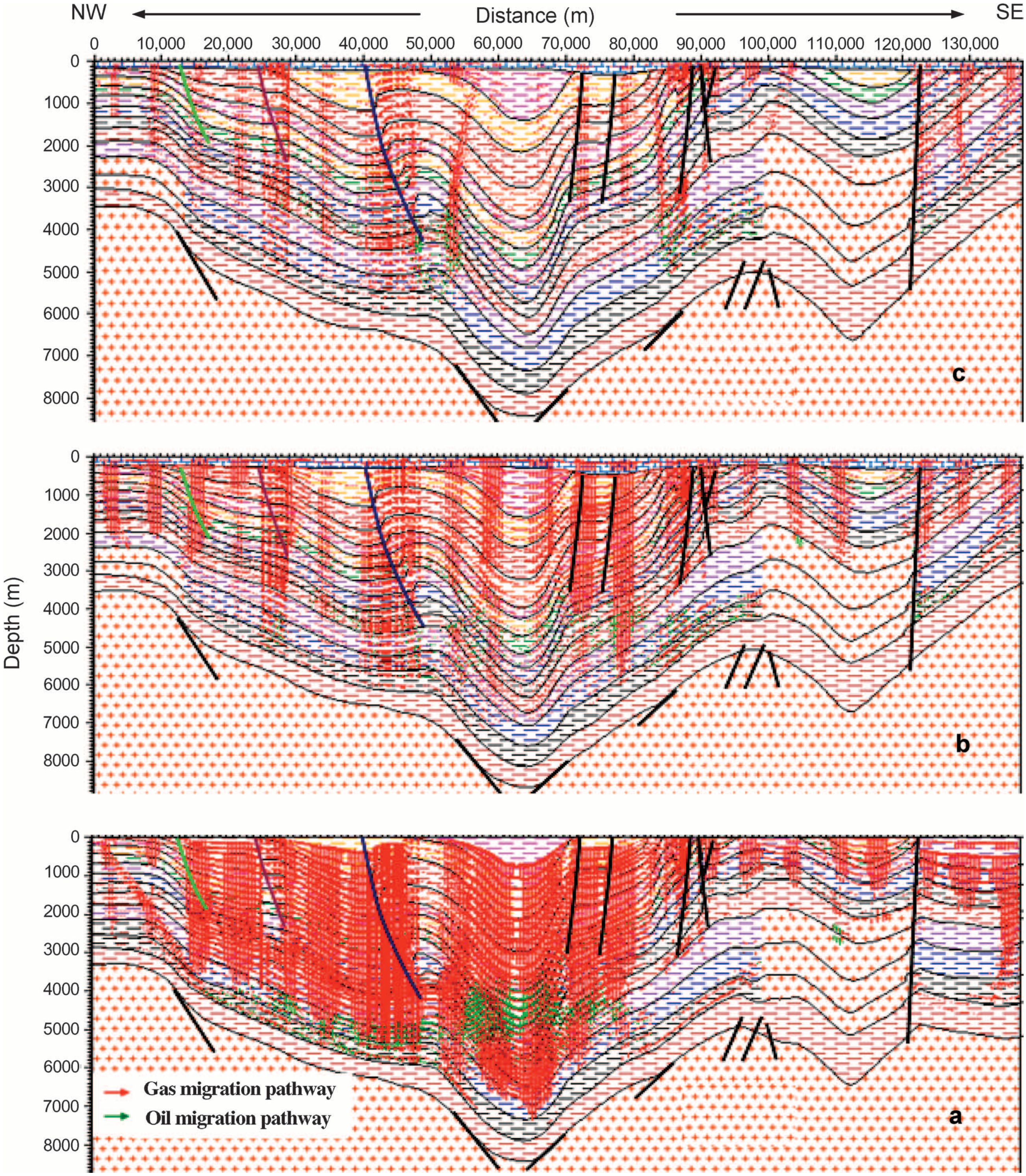

Figure 12. Model of petroleum migration in cross section S1 (oil shown in green, gas shown in red) during (a) the Carboniferous–Early Permian subsidence, (b) the Mesozoic, and (c) the Cenozoic time.

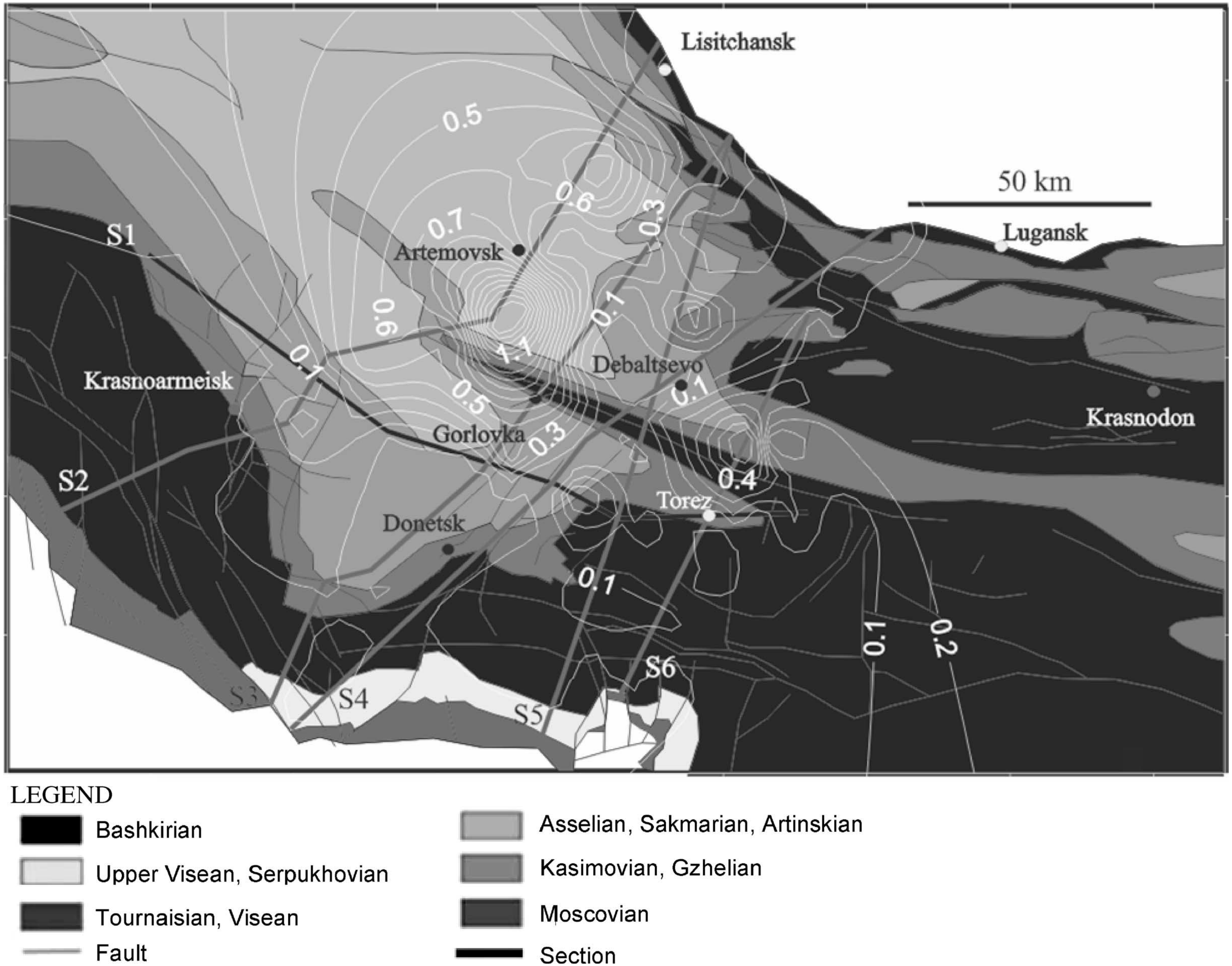

Figure 13. Predictive model of a natural gas trapped in the Donbas fold belt at a depth of 4 km (2 mi). Data are in trillion cubic feet (tcf).

predicted in the southern part close to the faults, in the zone of the main anticline, and in the northern part close to the fault and anticline with amounts of 0.2–0.5 tcf of methane. The methane reservoirs were simulated for all other cross sections to construct isomethane accumulation maps at a depth of 4 km (2 mi). Figure 13 shows that the higher amounts of trapped methane are located in the main and south synclines at a depth of 4000 m (13,123 ft) with an estimated maximum value of 2.0 tcf of methane. Two methane maxima are observed in the zone between Debaltsevo, Donetsk, and Torez, with methane accumulations of 0.2–0.8 tcf (Figure 13). The zone of meta-anthracite (southern and southeastern parts of Donetsk) is relatively poor in methane reservoirs (~0–0.3 tcf of methane).

The present study indicates that the overmature Carboniferous coal-bearing strata in the southeastern part of the DF contain virtually no preserved methane (Privalov et al., 2007). Stable C isotopic analyses suggest that CO_2 migrated from deep (mantle?) sources or magma chambers and replaced the methane (Privalov et al., 2004a). The formation of coalbed methane accumulations is suspected in less-mature Carboniferous coal-bearing strata (oil and gas window) and not sealed by Lower Permian rocks located between the Donetsk and Torez regions (Marshall et al., 1996; Radzivill, 1999; Privalov et al., 2004a; Privalov et al., 2007). Numerical simulation suggested that gas resources could be expected in the main anticline. This result matches with the distribution of known conventional gas deposits trapped in fractured and secondary reservoirs (Privalov et al., 2007). The 2-D basin modeling predicts methane accumulations in the main syncline, where Lower Permian seal rocks were preserved. However, it is important to keep in mind that the composition of gases is controlled by the regional hydrogeology (Scott et al., 1994; Scott, 2002; Pashin, 2007). The presence of secondary biogenic gases can be observed in conventional and unconventional gas deposits caused by bacteria introduced by meteoric waters (Scott et al., 1994; Ayers, 2002). Isotopic studies clearly indicated that the origin of methane in the DF is thermogenic (Belokon, 1987; Voitov et al., 1987; Privalov et al., 2004b). So, the northern flank of the study area may be considered as a viable prospective site for gas.

SUMMARY AND CONCLUSIONS

The geochemical analysis of coals in the DF indicates a significant source rock potential, with TOC values of coal seams ranging from 52 to 89% and HI values ranging from 210 to 310 mg/g TOC. Numerical basin modeling shows the following:

- Coal rank increases toward the eastern and southeastern parts of the study area (1) possibly because of an eastward increase in burial depth, (2) probably because of an eastward increase in HF, and (3) maybe because of magmatic activity observed in the southeastern part of the study area near Torez.
- A good fit was observed between simulated and measured vitrinite reflectance values by considering HFs of (1) approximately 40–75 mW/m^2 during the Carboniferous–Early Permian subsidence, (2) 120 mW/m^2 in the southwest of Donetsk caused by the intrusion of Permian alkaline rocks, and (3) 150 mW/m^2 in the south syncline and 130 mW/m^2 in the northern Krasnoarmeisk monocline caused by the Permian–Triassic magmatic events.
- A major erosional event occurred in the Late Permian with maximum total erosion in the southeastern part (~8 km, ~5 mi). Post-Permian erosions have had little effect on the coalification pattern.
- The main phase of hydrocarbon generation occurred during the Carboniferous–Early Permian subsidence. However, the Permian-Triassic magmatic events also induced pulses of hydrocarbon generation.
- Three phases of oil expulsion are predicted at (1) the Mississippian–Early Permian, (2) the Triassic–Jurassic, and (3) the Cretaceous.
- The uplift and erosion of sealing beds during the Late Permian and Late Cretaceous caused an intensive migration and dismigration of hydrocarbons.
- The presence of natural gas was confirmed in the south syncline and predicted in the main syncline,

where the Lower Permian salt-bearing sequences are preserved.

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