PETROLOGICAL AND GEOCHEMICAL CHARACTERIZATION OF CANDIOTA COAL SEAMS, BRAZIL – IMPLICATION FOR COAL FACIES INTERPRETATIONS

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Abstract– Seven coal seams, from cores of the borehole M-IV-C-101, Candiota Coalfield located in Rio Grande do Sul State, southern part of the Paraná Basin were analyzed by coal petrographical and organic geochemical methods. Results from petrographic analyses suggest deposition in open mires, with elevated contents of detrital macerals and clay minerals and also limno-telmatic coal facies. Results from geochemical analyses showed that terrestrial organic matter is predominant as indicated by hydrogen and oxygen indices, carbon preference indices and the sterane distribution. Geochemical maturity parameters such as the 20S/(20S+20R) and $\alpha\beta\beta/(\alpha\beta\beta + \alpha\alpha\alpha)$ ratios for C_{29} regular steranes support the low level of rank (maturity) as indicated by the vitrinite reflectance measurements (0.41-0.45%).

Keywords: Paraná Basin, Permian Coal, Organic Petrology, Organic Geochemistry, Coal Facies

1. Introduction

The Candiota coalfield is located in the southern part of Rio Grande do Sul, Brazil, and covers an area of approximately 2,000 km^2. The coal occurrences are assigned to the Rio Bonito Formation, a fluvial to marine sandstone and shale-prone unit of Early Permian age (Artinskian-Kungurian) (Fig. 1). In general, the Candiota coal seams are characterized by high ash yields in excess of 50 wt. %. The organic matter is intimately mixed with the mineral matter and a number of seams are characterized by relatively high liptinite and/or inertinite contents (Silva, 1994, 1999; Holz and Kalkreuth, 2004).

The aim of the present paper is to characterize coal seams from the Malha IV area of Candiota mine (seams Inferior 4 to 1, seam Camada Candiota Inferior, seam Camada Candiota Superior and the Banco Louco seam), based on coal petrographical and organic geochemical analyses, to further enhance our understanding of organic matter type, depositional environment and rank (maturity).

2. Methods

Petrographic analysis included maceral anlysis, microlithotype analysys, lithotype description and vitrinite reflectance measurement. Organic geochemical analyses included total organic carbon (TOC) determination, Rock-Eval pyrolysis, bitumen extraction and Liquid Chromatography, Gas Chromatography, and Gas Chromatography/Mass Spectrometry. TOC was analyzed using a WR-12 LECO Instruments carbon elemental analyzer, in which samples are heated at 1200 °C for 2 minutes under a constant oxygen stream. TOC was measured by a thermal conductivity detector and the result was reported as atomic weight (%). Rock-Eval pyrolysis was carried out according to Espitalié et al. (1977) procedures. Bitumen was extracted in a Soxhlet apparatus with dichloromethane as solvent, and the organic extracts were separated via liquid-column chromatography. The GC analyses of aliphatics were performed on a Varian 3700 chromatograph equipped with a split injector and fitted to a 25m x 0.33mm SE-54 column using hydrogen as carrier gas, with a temperature program of 40-280 °C/min. The GC-MS analyses were performed using a Varian 3700 chromatograph, A Varian 112-5 mass spectrometer coupled with a Varian 55-100-MS data acquisition system.

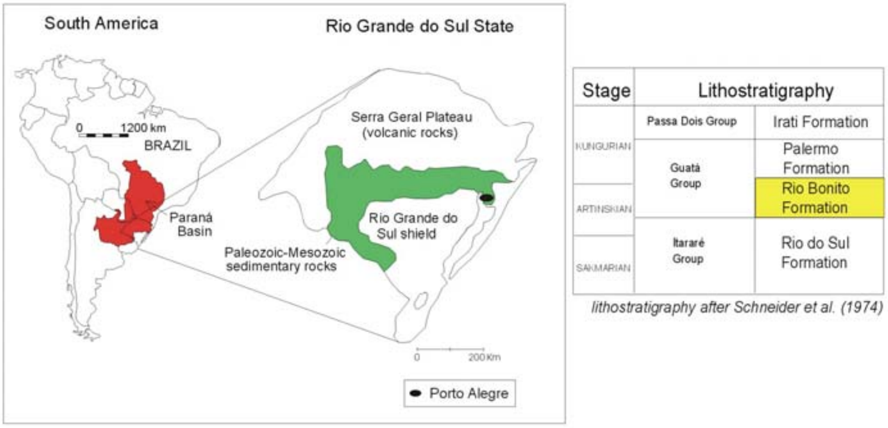

Figure 1: Location of study area and stratigraphic position of the coal-bearing Rio Bonito Formation.

3. Results

3.1. Petrology of Candiota Coal

Seams I4 and I2 are characterized by the highest contents of vitrinite group macerals and the lowest contents of mineral matter (Fig. 2). Seams I3 and I1 have the lowest vitrinite contents, whereas seam BL is extremely rich in inertinite (Fig. 2). CCI and CCS seams are characterized by roughly equal amounts of vitrinite and inertinite with only minor contribution from macerals of the liptinite group (Fig. 2).

Candiota coals are rich in mineral matter (Fig. 2), which consists mostly of clay-minerals, with minor contributions of quartz and pyrite. The majority of clay minerals occurs as organic matter-free layers, but occurs sometimes also in form of finely disseminated particles in vitrinite.

Random vitrinite reflectance measurements range from 0.41 to 0.45 %, similar to vitrinite reflectances of 0.37-0.44% reported in an earlier study (Silva, 1994).

3.2. Ternary Microlithotype Coal Facies Diagram

The facies diagram originally proposed by Hacquebard and Donaldson (1969) is based on four groups of microlithotype associations and suggests six coal facies environments (Fig. 3). The ternary diagram is actually subdivided into two parts: in the upper part, the dull component (D) constitutes less than 20% of the lithotype associations and is incorporated with component A at one corner of the triangle. In the lower diagram this component constitutes more than 20%, and when enriched in major concentrations are considered to indicate open-water moor facies.

The distribution of the microlithotype associations determined in the present study are shown in Figure 3, modified slightly from the original facies diagram of Hacquebard and Donaldson (1969). According to this figure open-water moor conditions are indicated for seams I3, I1, and BL, whereas CCS and CCI seams are located at the transition zone of an open-water/limno-telmatic forest moor. I4 and I2 seams have a microlithotype association indicating somewhat drier conditions within the limno-telmatic facies zone (Fig.3), characterized by the highest clarite contents and the lowest volumes of carbominerite and minerite.

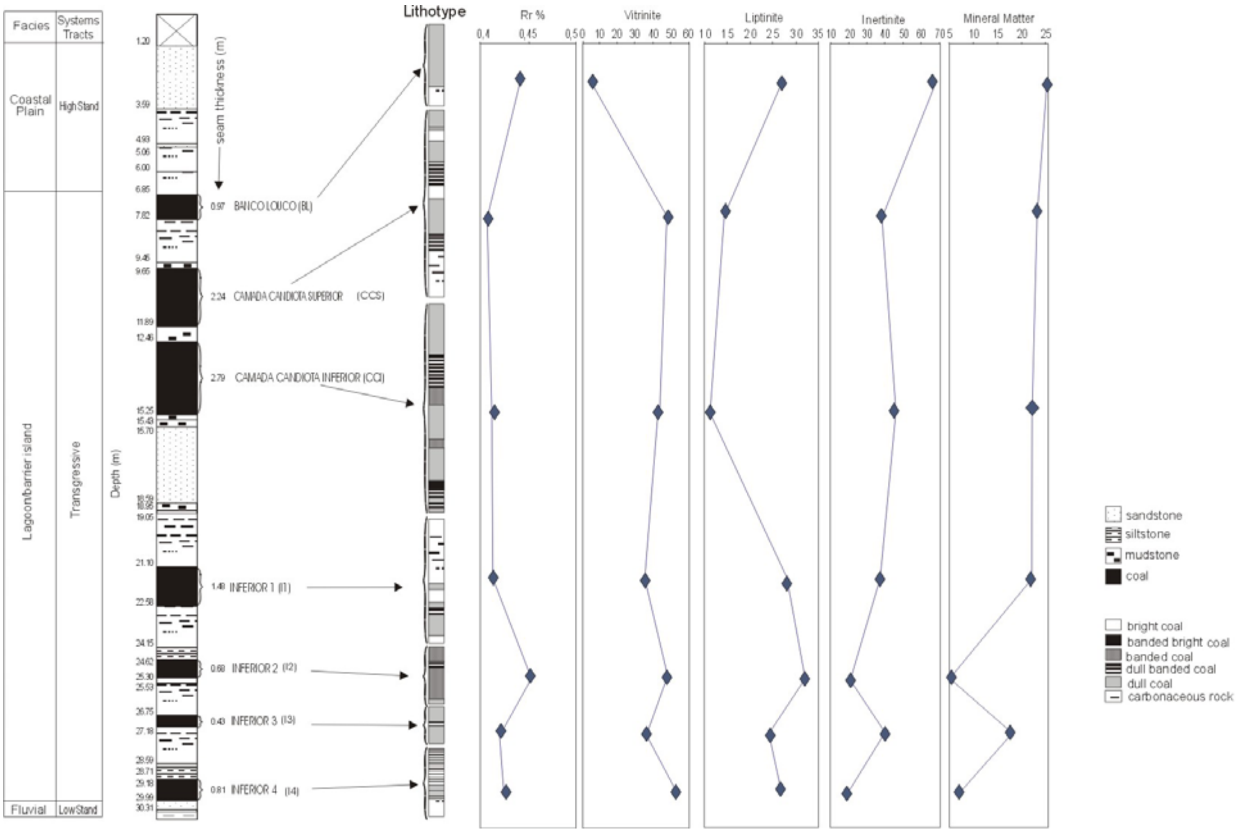

Figure 2: Lithological column of borehole M-IV-C-101, showing coal seam distribution and thickness, lithotypes, vitrinite reflectance values, maceral groups (Vol %, mineral matter-free basis), and mineral content (Vol %). Depositional setting of Candiota coal-bearing strata as suggested by Holz and Kalkreuth (2004).

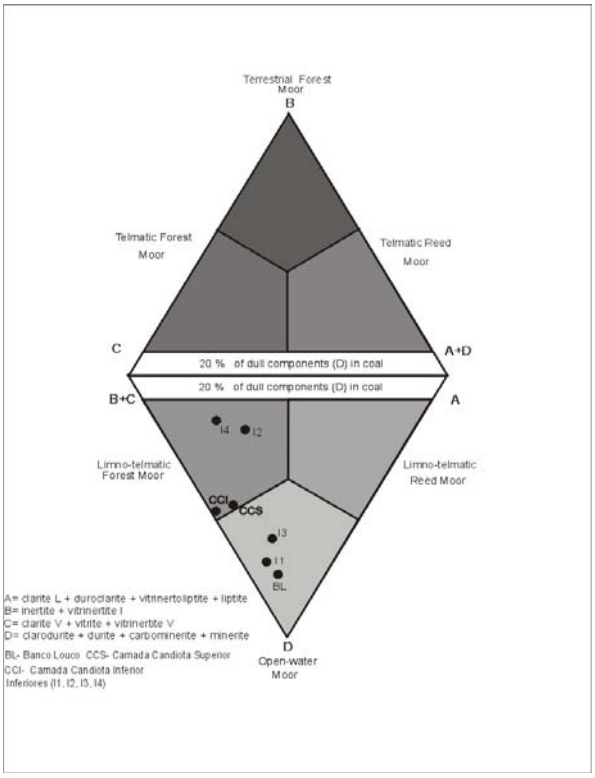

Figure 3: Four-component facies diagram for the coal samples from borehole M-IV-C-101, Candiota Mine, RS, Brazil (modified from Hacquebard and Donaldson, 1969).

3.3. Organic Geochemistry

3.3.1. TOC and Rock Eval Pyrolysis

TOC values are relatively low, ranging from 28 to 45 wt.%. Tmax values range from 428° to 436 °C suggesting a low thermal maturity and correspond to the low rank as indicated by random reflectance measurements. Figure 4 shows the relationship between hydrogen index, Tmax (°C), and kerogen types for Candiota coals.

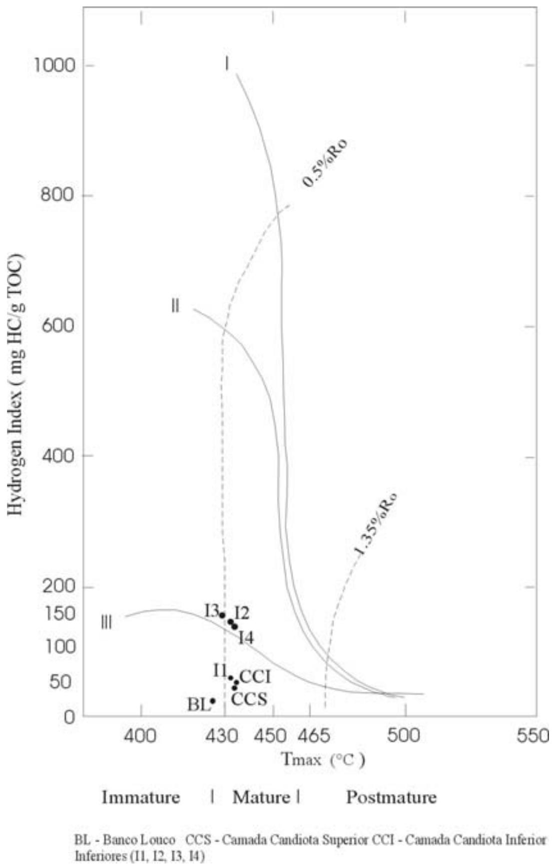

Figure 4: Diagram showing Hydrogen Indices and Tmax values for Candiota coals (modified from Mukhopadhayay et al., 1995).

3.3.2. Bitumen Extraction and Liquid Chromatography

In general, the bitumen extract content is low, ranging from 1222.8 to 4647.8 ppm. The lowest content of bitumen extract occurs in I3 seam, whereas the highest contents were identified in I4 and I2 coal samples. The I4 and I2 seams also have the highest contents in liptinite and vitrinite contents, as well as the lowest mineral matter contents. For the sample set analyzed there exists a trend of increasing extract yields with increasing vitrinite and liptinite contents (correlation coefficient r = 0.7258), and also a trend of increasing extract yields in relation to decreasing mineral matter contents (correlation coefficient r = 0.7583). The hetero (NSO) compounds predominate in the extracts of all samples, ranging from 50 to 62%.

3.3.3. GC Analyses

The n-alkanes of Candiota coal samples are dominated by long-chain n-alkanes (> n-C_{21}) with an odd over even predominance (CPI from 2.17 to 4.21), with the most prominent peaks at n-C_{25} in I3, I1, CCI, and CCS samples (Fig. 5) and at n-C_{27} in samples I4 and I2. The BL sample shows maximum intensities at n-C_{25} and n-C_{27} (Fig. 5).

A secondary n-alkane population occurs in the shorter-chain region (< C_{20}), particular in the chromatograms of samples CCS, BL and sample I3, suggesting a contribution of algae and microorganisms to the precursor peat. Alternatively, this population may also reflect a biodegradation of long-chain n-alkanes during peat accumulation (Peters and Moldowan, 1993).

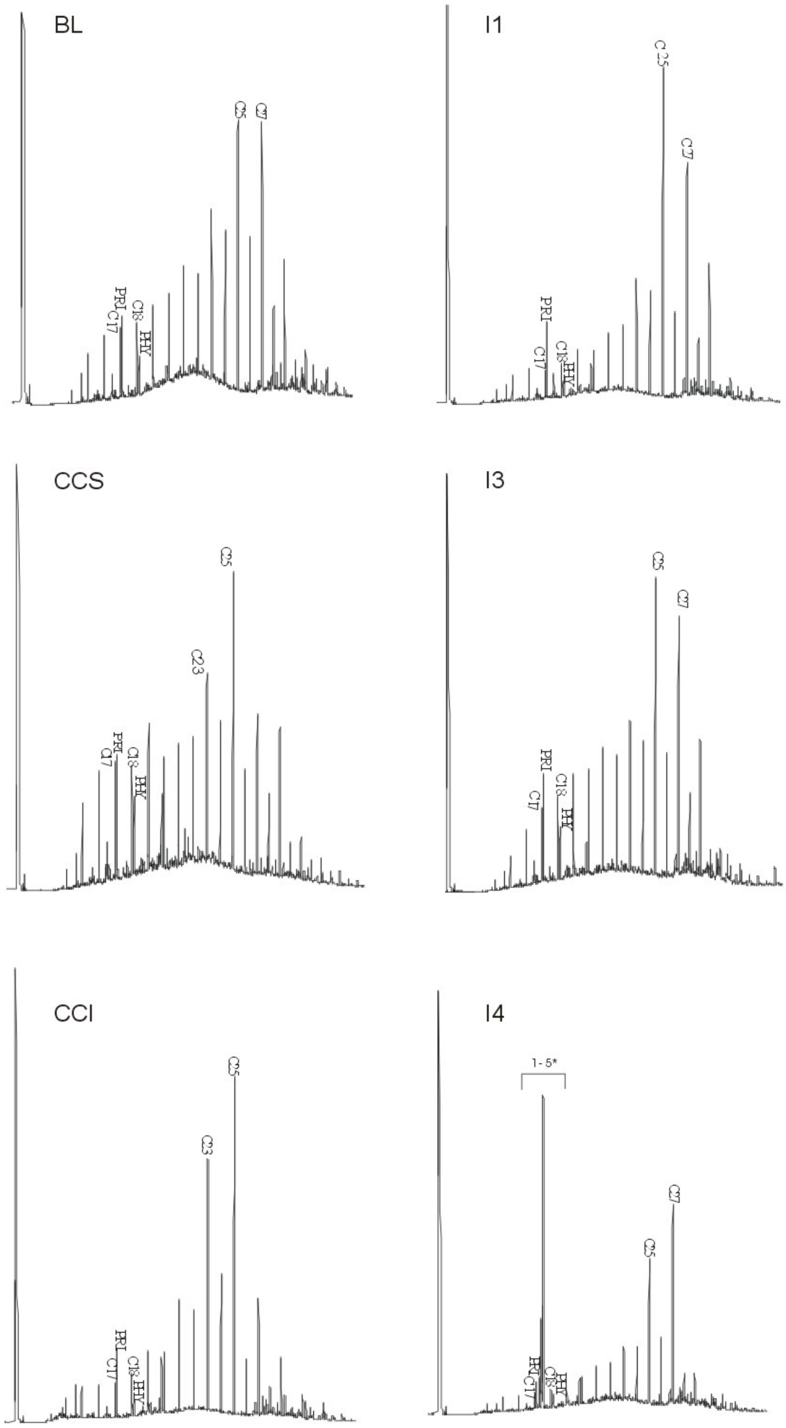

Figure 5: Gas chromatograms of saturated hydrocarbons of Candiota coal extracts. * new series of aliphatic and aromatic bicyclic compounds (Miranda et al., 1999). BL = Camada Banco Louco, CCS = Camada Candiota Superior, CCI = Camada Candiota Inferior, I1 = Camada Inferior 1, I3 = Camada Inferior 3, I4 = Camada Inferior 4

A family of bicyclic alkanes as described by Miranda et al. (1999) were also detected in relatively high abundance in the isoalkane/cycloalkane fractions of samples I4 and I2 seams. The position of these isoalkane/cycloalkane fraction is shown for seam I4 in Figure 5. These bicyclic hydrocarbons have been interpreted to relate to a common biological precursor, possibly a conifer resin-derived tricyclic diterpenoid (Miranda et al., 1999).

The pristane (Pr)/phytane (Ph) - ratio is considered to be an indicator of relative oxic or reducing environments during early diagenesis, with suboxic to oxic environments characterized by Pr/Ph - ratios >1 (Peters and Moldowan, 1993). Candiota coal samples show Pr/Ph - ratios ranging from 1.49 to 4.47 thus indicating a certain level of oxygen access to the site of peat accumulation.

3.3.4. GC/MS Analyses

Regular steranes are biomarkers considered to indicate organic matter sources that contributed to the organic portion of the sediment. A predominance of C_{29} steranes is related to a strong terrestrial contribution, whereas a predominance of C_{27} and C_{28} indicate a predominance of marine phytoplankton and lacustrine algae, respectively (Waples and Machihara, 1991). The relationships are complicated by the known fact, that the C_{29} sterane also occurs in certain brown and green algae.

In the Candiota samples the proportions of C_{29} steranes (44-49%) are highest, followed by C_{27} steranes (30-34%) and C28 steranes (20-22%). Although the C_{29} steranes are predominant, even a higher contribution had been expected since typically humic and waxy coals display a strong dominance of C_{29} steranes (Waples and Machihara, 1991). The relatively high C_{27} and C_{28} sterane proportions suggest a contribution of algae, bacteria and possibly fungi to the precursor peat. The C_{29} sterol chain may also have been degraded by bacteria (Piedad-Sánchez et al., 2004), which is supported by the relatively high contents of degraded collodetrinite in the Candiota coal seams.

Biomarker ratios such as the 20S/(20S+20R) and αββ/(αββ + ααα) for C_{29} regular steranes and the ratio of tricyclic triterpanes to pentacyclics (TRI/HOP) are used in petroleum exploration to evaluate maturity levels of the organic matter and are used here to confirm the low rank of Candiota coals as determined by vitrinite reflectance measurements.

4. Conclusions

Maceral Composition and Mineral Matter. The organic matter in the Candiota coals is dominated by macerals of the vitrinite and inertinite groups. Despite a significant scatter in the data points, a general increase of inertinite is indicated from the base to the top of the coal-bearing sequence, whereas vitrinite contents decrease. Liptinite contents vary from 11 to 32 Vol%, with microsporinite and liptodetrinite being the most abundant liptinite macerals. Mineral matter ranges from 5 to 25 Vol % and is dominated by clay minerals.

Coal Facies Interpretation. The coal facies model based on microlithotype distribution suggests that the Candiota peat accumulated under high water tables under a reothrophic regime (transition to open mire facies).

Geochemical Analyses. Results from Rock Eval analyses, CPI and biomarker distribution (C_{27}, C_{28}, C_{29}) indicate a predominance of terrestrial organic matter, although the presence of lower chain alkanes (< C_{20}) and the relatively high proportion of C_{27} steranes suggest also some contribution of algae or bacterial source organic matter. The Pr/Ph ratios are relatively high, suggesting a suboxic/oxic environment of deposition. Biomarker ratios such as the 20S/(20S+20R) and αββ/(αββ + ααα) for C_{29} regular steranes confirm the low maturity of the organic matter as determined by vitrinite reflectance. (0.41-0.45%).

5. References

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