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Coal modeling using Markov Chain and Monte Carlo simulation: Analysis of microlithotype and lithotype succession

Saeid R. Dindarloo [a], Amirhossein Bagherieh [a], James C. Hower [b,*], John H. Calder [c], Nicola J. Wagner [d,1]

[a] Department of Mining and Nuclear Engineering, Missouri University of Science and Technology, Rolla, MO 65409-0450, USA
[b] University of Kentucky, Center for Applied Energy Research, 2540 Research Park Drive, Lexington, KY 40511, USA
[c] Nova Scotia Department of Natural Resources, Halifax, Nova Scotia B3J 3K5, Canada
[d] University of the Witwatersrand, Johannesburg, South Africa

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ABSTRACT

Markov Chain analysis was applied to the description of the megascopic lithologic transitions in Pennsylvanian-age eastern Kentucky coals. Coal lithology modeling can be problematic as individual lithotypes can represent near-instantaneous events (vitrain), prolonged degradation (durain), or fire-induced loss of previously deposited lithologies (fusain). Each of the latter lithotypes, potentially representing vastly different amounts of time, could be of the same thickness. Therefore, equal thickness does not necessarily imply equal time. Probability transform matrices that employ uniform lithotype thicknesses were used, allowing transitions between like lithotypes; embedded Markov Chains, thereby only considering transitions between different lithotypes; and continuous-time Markov Chains were employed in the assessment of a section of the No. 5 Block coal (Pennsylvanian Breathitt Group, Martin County, Kentucky). Embedded Markov Chains could successfully simulate the lithologic transitions. A Monte Carlo random process was programmed to simulate thickness variations of lithotypes between the transitions. The proposed hybrid model of Monte Carlo–Markov Chain was able to predict the random pattern that underlies lithotypes transitions and thickness. The hybrid Monte Carlo–Markov Chain technique proved to be effective in the case study in simulating both the lithologic thickness variations and transitions.

1. Introduction

In the petrographic order of coals, lithotypes are the macroscopic expression of microlithotypes which, in turn, are the microscopic assemblages of macerals and minerals (Hower et al., 1990; Taylor et al., 1998; Esterle, 2008; Hower and Wagner, 2012; O'Keefe et al., 2013). Microlithotypes, ideally representing assemblages at least 50-μm thick, are defined based on the relative proportions of macerals and minerals present in the interval (Table 1). Microlithotypes, even more than the macerals comprising the assemblage, represent the first-order approximation of coal depositional conditions. As discussed by O'Keefe et al. (2013) and Hower et al. (2013), the path from wood to vitrinite and inertinite can be quite complex and involve the actions of insects and other fauna, fungus, and bacteria. The succession and the thickness of lithotypes and the constituent macerals and microlithotypes determine the mining and handling properties of coal (Hower and Lineberry, 1988; Hower, 1998, 2008).

Coal lithotypes, all basically combinations of vitrain, durain, and fusain (and thin mineral-rich bands) are defined on the basis of a 3-mm minimum thickness,[2] represent variable times for their deposition, making it difficult to prescribe exact rules to lithotypes succession. For example, a vitrain, usually a thin (mm to a few cm) lithotype, may represent a well-preserved part of a log, branch, or root; overall, a short time in the history of the coal. Prior to the incorporation of the plant part into the peat, the wood may have been attacked by insects, perhaps before or after an infestation of fungus (Hower et al., 2013). Post-depositional microbial attack may further alter the lithotype. In contrast, fusain, also generally a thin lithotype, in the classic sense could represent a fire event (Stach, 1927; Evans, 1929; Scott, 1989, 2000, 2002; Winston, 1993; Scott and Jones, 1994; Guo and Bustin, 1998; Petersen, 1998; Bustin and Guo, 1999; Scott et al., 2000; Scott and Glasspool, 2005, 2006, 2007; McParland et al., 2007). As such, fusain potentially represents an unknown span of time, which may be an unconformity within the coal bed. Durains can represent a longer span of time, from decay in a standing tree, to degradation in the peat surface litter, to subsurface aerobic (fungal and bacterial) and anaerobic (bacterial)

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[2] The bright clarain, clarain, and dull clarain lithotypes are fundamentally alternating vitrain and durain, each of the latter two being too thin to separate into the basic units. An attempt is made to recognize thinner fusains and inorganic partings because they represent a significant disruption in the organic deposition.

* Corresponding author. Tel.: +1 859 257 0261.
E-mail address: james.hower@uky.edu (J.C. Hower).

[1] Now at University of Johannesburg, Johannesburg, South Africa.

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Table 1
Maceral group composition of microlithotypes.

Microlithotype	Maceral group
Monomaceral	
Vitrite	Vitrinite (V) >95%
Liptite	Liptinite (L) >95%
Inertite	Inertinite (I) >95%
Bimaceral	
Clarite	V + L > 95%
Vitrinertite	V + I > 95%
Durite	L + I > 95%
Trimaceral	
Duroclarite	V > L, I (each >5%)
Clarodurite	I > V, L (each >5%)
Vitrinertoliptite	L > V, I (each >5%)
Carbominerite	Coal + 20–60% (vol.) clays Coal + 5–20% (vol.) sulfides

degradation (Stach, 1927; Duparque and Delattre, 1953a,b; Belkin et al., 2009, 2010; Hower et al., 2009, 2011a,b, 2013; Loo, 2009; O'Keefe and Hower, 2011; O'Keefe et al., 2011, 2013). Therefore, in defining succession of lithotypes, transitions between distinct lithotypes and the continuum of thick individual lithotypes each represent different forms of the same process, the time- and space-dependent growth of the peat deposit.

Sequences of lithotypes and microlithotypes are assumed to have a stationary (homogeneous) first-order Markovian properties (Markov, 1906). In this study, we test the Markov properties of a lithotype succession from the No. 5 Block coal of eastern Kentucky and a microlithotype succession from the Kimberly Middle Split coal from Joggins, Nova Scotia, Canada to examine applicability of Markov chains and Monte Carlo methods in modeling both the coal (micro) lithotypes transitions and thicknesses.

Eastern Kentucky coals, including the No. 5 Block coal investigated here, typically have complex lithologic profiles, tending to have a high frequency of thick, dull, liptinite- and inertinite-rich lithotypes (durain; known locally as splint) (Hower et al., 1994; Richardson et al., 2012). The Langsettian (Westphalian A) Kimberly Middle Split coal, as with many of the coals exposed at Joggins, Nova Scotia, was deposited in a planar mire dominated by lycopsid trees and tree ferns (Hower et al., 2000).

2. Methods

Table 2
Tally Frequency Matrix for the No. 5 Block coal, showing the number of transitions between all states.

	Clarain	Vitrain	Fusain	Durain	Clay	Dull clarain	Bright clarain	Total
Clarain	147	9	6	4	1	1	1	169
Vitrain	9	38	0	0	0	0	0	47
Fusain	6	0	12	0	0	0	0	18
Durain	4	0	0	317	0	1	0	322
Clay	1	0	0	0	179	0	0	180
Dull clarain	2	0	0	0	0	113	0	115
Bright clarain	1	0	0	0	0	0	89	90
Total	170	47	18	321	180	115	90	941

Table 3
Limiting probability matrix of the No. 5 Block coal.

	Clarain	Vitrain	Fusain	Durain	Clay	Dull clarain	Bright clarain
Clarain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Vitrain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Fusain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Durain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Clay	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Dull clarain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234
Bright clarain	0.4912	0.2105	0.1404	0.0702	0.0234	0.0409	0.0234

Markov chain analysis is a simple, powerful mathematical technique that may enable geologists to employ a quantitative approach to stratigraphic problems that have previously been dealt with rather subjectively (e.g., Lumsden, 1975). A Markov chain is a sequence or chain of discrete states in time (or space) in which the probability of the transition from one state to a given state in the next step in the chain depends only on the previous state (Harbaugh and Bonham-Carter, 1970). A Markov chain transition probability P_{ij} is a conditional probability defined by Eq. (1):

$$P\{X_{n+1}=j|X_n=i,\ X_{n-1}=i_{n-1}\ldots X_1=i_1, X_0=i_0\} \\ = P\{X_{n+1}=j|X_n=i\}=P_{ij} \tag{1}$$

where, n is the time step, i and j are system states, and P_{ij} is the probability of transition from state i to state j in the next time step (Ross, 2010).

From the definition, it is obvious that the following conditions should be met:

$$P_{ij} \geq 0, \quad i,j \geq 0; \ \sum_{j=0}^{\infty} P_{ij}=1, \quad i=0,1,\ldots. \tag{2}$$

In a homogeneous Markov chain, as in this study, P_{ij} is the same for all n. The properties of Markov chains are intermediate between totally random and totally deterministic sequences of events (Lumsden, 1975). In this study, prediction and simulation of a succession of lithotypes in a coal bed are an area which well fits the definition and mathematical power of Markov chain analysis; lithotype succession follows some expected patterns based on evolution of the depositional environments, but they do not represent instantaneous events and the consequent time factor serves to complicate the nature of the lithotypes, thereby complicating the succession. The literature on Markov Chain analyses of lithological succession is now rapidly growing, with test cases published by Harbaugh and Bonham-Carter (1970), Smyth and Cook (1976), Khan and Casshyap (1982), Tewari and Casshyap (1983), Mack and James (1986), Smyth and Buckley (1993), Carle and Fogg (1990, 1996), Sharma et al (2001), Hota and Maejima (2004), Tewari et al. (2009), and Hower et al. (2011c). Applicability of the technique will be discussed in the following sections through the consideration of several coal layers.

2.1. Analysis of the lithotypes

The lithologic description of the No. 5 Block coal by Don Pollock and Eric Trinkle (personal communication to Hower, 1983) followed the procedures later outlined by Hower et al. (1990).

Table 4
Entropy values for Kimberly Middle Split coal.

Microlithotype	E Post	E Pre
Carbominerite	1.822	2.978
Vitrite	2.172	4.448
Liptite	0.918	0.326
Inertite	1.790	1.444
Clarite	2.190	3.166
Vitrinertite	2.189	1.277
Durite	1.585	0.301
Duroclarite	2.464	3.837
Clarodurite	1.842	0.807
Vitrinertoliptite	1.500	0.869
Clay	0.000	0.528