[PS]Potential to Generate Oil Prone Coal Source Rocks in Arctic Environments*

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Abstract

Using knowledge of productivity, decay and atmospheric deposition we demonstrate that latitudinal and geographic variation in low ash coal composition can be predicted and that a warm arctic is an ideal environment in which to produce hydrogen-rich/oil prone coal. This coal, a type III kerogen source rock, has specific properties; a high proportion of microbial aliphatic compounds indicative of aerobic decay; sufficient sulfur (>1 wt %) to crosslink and stabilise aliphatic compounds within the coal. It is recognised that these properties are produced in coastal settings, however a more fundamental control on the oil potential of coals are latitudinal gradients in the balance between productivity and decay. This balance determines the long term carbon accumulation rate of the precursor peat, the potential for aerobic decay and ultimately the balance between atmospherically deposited sulphur and aliphatic compounds within the coal.

An initial model is created using known latitudinal variation in peat carbon accumulation rate, depositional rates of mineral dust and sulfur and the carbon loss during coalification, derived from the van Krevelen diagram for type III kerogen. Using this model, graphs illustrating elemental concentration vs. coal rank are contoured for latitudinal change in peat carbon accumulation rate. To test the model we compare predicted Ti and S concentrations in low, mid and high latitude Paleocene coal taken from South America, North America and the Arctic region respectively. These regions were selected as their palaeogeography has remained remarkably stable since the Paleocene.

A good correlation is observed between predicted and measured Ti and S concentrations. Sulfur concentrations exceeding 1% (required for oil prone coal formation) are generated at high latitude from low sulfur deposition rates in the range 0.1 to 0.2 g(S) m-2 yr-1 whereas in tropical peat deposits these concentrations will only be reached with deposition rates > 1 g(S) m-2 yr-1, found only in coastal environments. In addition to high sulfur concentrations, high rates of decay are also required to generate lipid rich peat. Under cold climatic conditions decay rates and net

primary production (NPP) are low. The effect of warming is to increase both NPP and decay rate however respiratory decay rates increase more rapidly than NPP with increasing temperature, favouring the generation of typical microbial lipids. In winter if soil temperatures remain high, decay rates will be high, but productivity will be suppressed due to low light levels. Estimates of Paleocene palaeobotanical ecosystem productivity are equivalent to those of temperate forests and this is consistent with both elevated NPP and decay. We conclude that warm arctic palaeoenvironments are ideal for the generation of oil prone, hydrogen rich coal source rocks.

Potential to Generate Oil Prone Coal Source Rocks in Arctic Environments

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1) Introduction

Oil prone coal, a type III kerogen source rock, has specific properties; a high proportion of microbial aliphatic compounds indicative of aerobic decay; sufficient sulfur (generally >1 wt %) to crosslink and stabilise aliphatic compounds within the coal (Sandison et al 2002). Consequently oil prone coal occurs in paralic settings, where the influence of seawater can provide the required sulfur and raise the pH of the peatland favouring rapid humification and the easiest way of achieving this influence is via marine aerosol deposition. At a more fundamental the influence of marine aerosol will be determined by latitudinal gradients in the balance between productivity and decay. This balance determines the long term carbon accumulation rate of the precursor peat, and consequently the ratio of sea salt and sulfur to organic matter within the coal.

2) Approach and Method

For elements provided to peat via atmospheric deposition it should be possible to predict variations in the composition of the subsequent lignite and coal if systematic changes in the following are known:

1.Latitudinal gradients in long term carbon accumulation rate
2.Rate of atmospheric deposition
3.Loss of mass during coalification

To illustrate that this approach can work we will first illustrate that it can be used to predict global trends in the Ti concentration of Cenozoic coal. We will then apply the same approach to predicting global patterns in the influence of marine aerosol deposition on paralic coal deposits and hence the extent of oil prone coal.

Ti is an ideal element on which to test our approach as it is supplied to peat via atmospheric deposition of mineral dust and has a low solubility therefore the amount of Ti is not easily modified post-deposition. Sulfur entering the peat via atmospheric deposition is also largely retained either as pyrite or organic S (Moore et al 2005).

2.1 Latitudinal gradients in long term carbon accumulation in peatland
Holocene long term carbon accumulation rates were compiled and plotted (Figure 1). Only data for complete peat profiles in which age, peat density and carbon concentration were measured are used. This greatly reduces the size of the available dataset (Yu et al 2010) , which is extended by inferring density and carbon concentrations for dated peat profiles. We consider this assumption to be invalid as the as the density of peat, particularly tropical peat varies markedly (0.2 to 0.025 g/cm3) even within a single profile (Page et al 2004). The results (Figure 1) illustrate a decrease in long term carbon accumulation rate from low to high latitude and a simple linear fit to this data was used to predict carbon and hence organic matter accumulation rates.

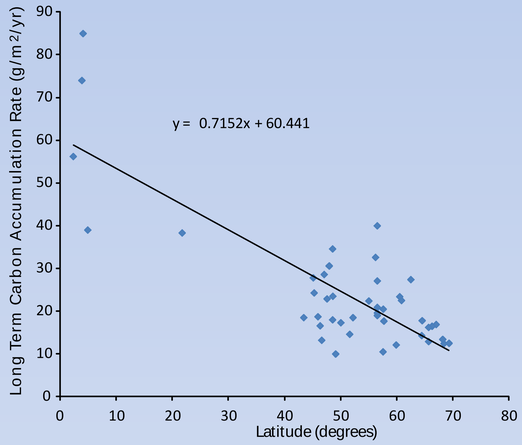


Figure 1. Long term carbon accumulation rate in Holocene peat vs latitude. Linear trend and associate equation used to estimate Cenozoic carbon accumulation rates is shown.

2.2 Mass loss during coalification.
This is estimated by assuming that mass loss during coalification on a dry basis from peat to low rank bituminous coal primarily involves the loss of CO2 and CH4 from organic matter in the general stoichiometric relationship $C_2H_4O_2 \Rightarrow CO_2 + CH_4$. and at higher ranks a shift to losing H_2O. Although not strictly correct this assumption reproduces the coalification trend on a van Krevelen diagram. (Figure 2) and therefore is assumed to adequately account for the mass loss during coalification.

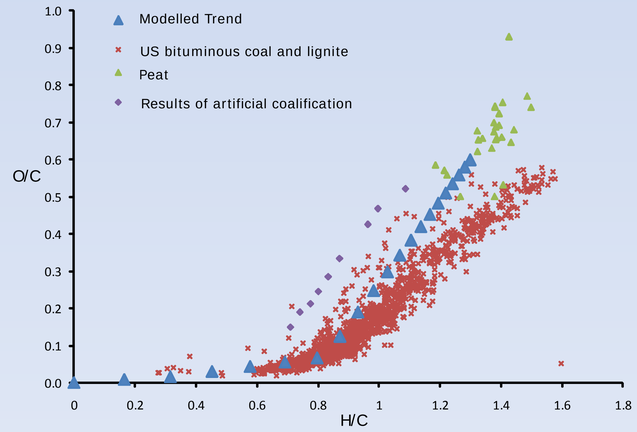
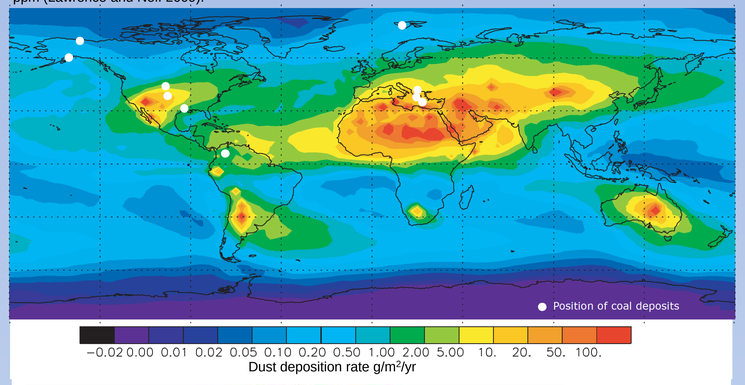


Figure 2. The trend used to predict mass loss during coalification plotted on a van Kevelen diagram and compared to the USGS coals (Bragg et al 1998), peat (Klavins et al 2008), and the result of artificial coalification (Mursito et al 2010).

3) Testing the approach – Predicting Ti concentration in coal.

To test whether this approach can be used to predicted Ti concentrations Cenozoic coal seams were chosen from South America (Martinez et al , 2001), North America (Bragg et al 1998), Svalbard (Orheim et al 2007)and Southern Europe (Papanicolaou et al 2005), regions for which the palaeogeography and palaeolatitude has remained similar throughout the Cenozoic. (Figure 3) The coal deposits were also selected to span a wide range latitude and inferred dust deposition rate (Figure 3).

Atmospheric deposition of Ti is in the form of mineral dust. With the current continental configuration and climate the highest dust deposition rates occur in continental interiors at tropics, and lowest deposition rates at high latitude and close to the equator. We assume this pattern would have been similar for areas with similar continental configuration throughout the Cenozoic. Predicted mineral dust deposition rates were taken from Mahowald et al 2006a (Figure 3) Ti concentration in mineral dust is taken as 5000 ppm (Lawrence and Neff 2009).



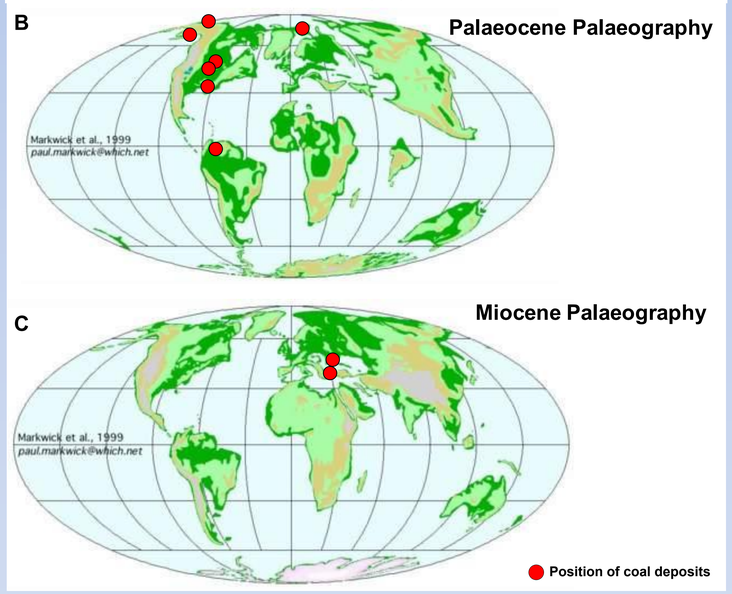


Figure 3. Position of coal seams selected for Ti concentration prediction relative to A) predicted recent mineral dust deposition rates (Mahowald et al 2006), B) Paleocene palaeogeography (Markwick et al 2000) and C) Miocene palaeography (Markwick et al 2000).

4) Predicted vs. measured Ti concentrations

Predicted vs. measured Ti concentrations (Figure 4) display good agreement . This is interpreted as indicating that the underlying assumptions used to calculate mineral matter deposition are reasonable and applicable to the Cenozoic. The one notable outlier are deposits from New Mexico and this may indicate that this area was less dusty in the Paleocene.

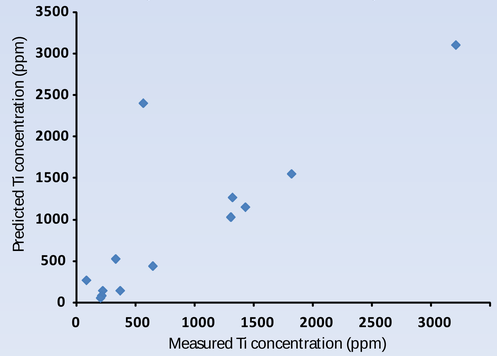


Figure 4. Measured vs maximum predicted Ti concentrations in Cenozoic coal.

5) Predicting sea salt sulfur deposition

Sea salt deposition will only make a significant contribution to total sulfur deposition in coastal areas. Maximum coastal sea salt deposition rates are typically 20 g/m²/yr of which 0.51 g/m²/yr is S compared to inner continental values of sea salt deposition of < 1 g/m²/yr of which < 0.025 g/m²/yr will be S (Mahowald et al 2006b).

Rates of deposition of sea salt and sea salt sulfate decrease rapidly inland (Gustafsson 2000, Mahowald et al 2006b). The sea salt sulfate deposition rates used in this study to calculate coal composition are derived from an empirical formula for sea salt deposition $y = 1.0941x^{-0.5527}$ (Hossain and Easa 2011) where x is distance in kilometres, and y sulphate deposition rate in mg/m²/d. Total sulphur deposition will be higher than this as it will include many non-seasalt sulfur species and to account for this a general low atmospheric background value of 0.02 g/m²/yr, typical of a low pre-industrial rate ((Stevenson et al 2003), is added to the sea salt sulfur deposition rate. The total amount of sea salt sulfur deposited will also depend on wind velocity and the salinity of coastal waters both of which are unknown at the time of coal deposition. Finally it is assumed that 75% of sulfur entering the peat is retained (Moore et al 2005). No account is made for S loss during coalification, but as coal rank does not change on the scale of observation we do not believe this will have a significant effect.

6) Predicted sulfur concentrations

The sulfur concentration expected in paralic bituminous coal in transects in from the coast is calculated for high, mid, and low latitude (Figure 5) bituminous coal containing 78% carbon on a dry ash free basis. As expected the S concentration decreases inland and is lower in the rapidly accumulating tropical coal deposits and higher in the slowly accumulating high latitude coal. If 1% S is taken as an indicator of the influence of marine aerosol and the likelihood of forming a significantly oil prone coal then at high latitude the region of oil prone coal formation extends 4 km inland from the coast and at low latitude only 0.1-0.2 km (Figure 5).

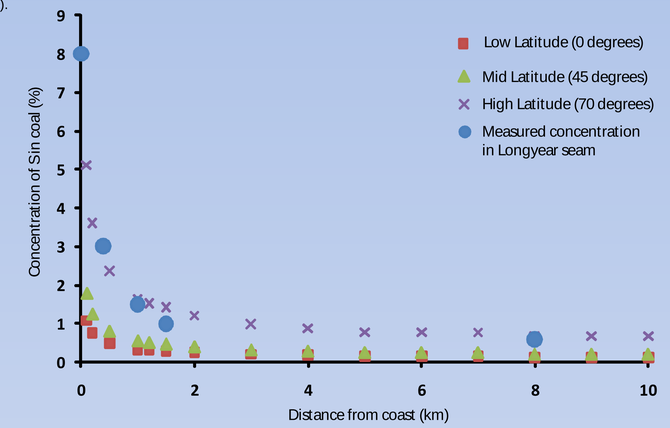


Figure 5 Predicted low, mid and high latitude trends in the sulphur concentration in bituminous coal going inland from the coast compared to the measured concentrations in the Paleocene high latitude Longyear seam.. The minimum inland concentration in the Longyear seam is taken from Orheim et al 2007 and set at 8 km, other values are taken from mine data and distances are measured relative to a mudstone-coal transition.

7) Comparison of Predicted and Observed S concentrations.

It is difficult to find values in the literature with which to compare predicted trends. Many reported values are for whole seams, or the palaeogeographic position relative to the coast is not well constrained. The comparison used here is from the Longyear seam a oil prone bituminous arctic coal from Svalbard, with 78% carbon measured on dry ash free basis. Distance from the coast was measured as distance from a mudstone – coal transition interpreted to have been the boundary between peat and coastal mudflats. The measured S data display similar trends and the comparison of absolute values is also extremely good. Most importantly the similarity between predicted and observed trends may indicate that the model is providing a reasonable prediction.

8) Conclusion regarding high latitude oil prone coal

The models used in this study appear to provide a remarkably good prediction of the influence of atmospheric deposition on Cenozoic coal composition. Results demonstrate that because of the lower carbon accumulation rates at high latitude the influence of marine aerosol and consequently the conditions suitable for the formation of oil prone coal are likely to extend many kilometres further inland from the coast. Conversely for coal deposited in tropical environments the zone of marine influence and oil prone coal formation is likely to be confined to within a few hundred meters of the coast.

Marine aerosol and sulfur supply alone are unlikely to produce oil prone coals in the absence of rapid decay. Under cold arctic conditions both decay and peat production will be negligible. The effect a warm arctic will be to increase both peatland productivity and the rate of decay. Respiratory decay rates increase more rapidly than vegetation productivity with increasing temperature (Fierer et al 2005), so in the arctic if soil temperatures remain high, decay rates will be high and sustained throughout the year even when productivity is suppressed due to low light levels. It is therefore concluded that the combination of the widespread influence of marine aerosol and a warm arctic palaeoenvironment will be optimal for the generation of oil prone coal.

We have therefore shown using knowledge of peat accumulation and atmospheric deposition that latitudinal and geographic variation in coal composition can be predicted and that a warm arctic should be an ideal environment in which to produce extensive oil prone coal.

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