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Organic Facies Prediction Model

Getech, Kitson House, Elmete Hall, Elmete Lane, Leeds LS8 2LJ, UK
Getech Inc., 3000 Wilcrest Dr. Suite 155, Houston, TX 77042, USA
UK. +44 113 322 2200 USA. +1 713 979 9900 info@getech.com www.getech.com

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Introduction

The ability to establish areas where organic-rich sediments may have been potentially deposited in the past is a fundamental aspect of the exploration workflow. The risks associated with accurately predicting source rock presence and quality are determined ideally by detailed analysis of observed data; however, these data are often lacking, especially in frontier areas. In the absence of such data, theoretical predictive models can play an important role.

The Organic Facies Prediction (OFP) Model was developed for predicting the initial (pre-maturation) total organic carbon (TOC) content and hydrogen index (HI) of sediments. It was designed to work anywhere with minimal data so that it could be of value in frontier exploration areas where information is sparse or where limited/clustered data make interpolation and extrapolation difficult.

Background to the IPD Modelling Concept

To calculate the initial organic content of sediments, we need to know the supply of organic matter (OM; input), the extent to which that supply has been preserved and the degree to which the remainder has been diluted by inorganic sediment. Some refer to this triumvirate as "production, destruction and dilution", or "productivity, preservation and sedimentation rate", but we believe that input, preservation and dilution (IPD) is more precise (Tyson, 2005). All three terms are always required to calculate a TOC value:

TOC% = ((Input x Preservation)/(Input x Preservation x OM Factor) + Mineral Dilution) x 100

Equation 1

which is equivalent to:

TOC% = OCAR/(OMAR + omfMSAR) x 100 *Equation 2*

where OCAR is organic carbon accumulation rate, OMAR is organic matter accumulation rate and omfMSAR is the organic-matter-free mass sediment accumulation rate.

The grain size effect on TOC that is not specifically represented in this equation comprises elements of input (co-deposition of mud and OM in low-energy areas), preservation (sediment permeability and its effect on oxidant supply, etc.) and dilution (surface area: volume versus particle size).

The input and dilution terms in the TOC equation are absolute fluxes and are deposited in units of mass/unit area/unit time (g/m2/yr in modern environments). The preservation term is just a percentage. The OM factor term is OM%/TOC% because OM (mainly C, H, and O) is what is added to the sediment but its abundance is expressed in terms of just the carbon. Of the three terms, dilution (or the OM/mineral ratio) is the most neglected, despite its global range (and thus potential impact) being significantly greater than that of productivity. TOC is definitely not just about the productivity or preservation of the organic fraction, even though these terms have historically received most of the attention.

The input term is not productivity. The largest losses of carbon always occur before planktonic OM enters the sediment as the particulate OM is partially degraded (and/or solubilised) when it sinks through the water column. Most planktonic OM (80% or more) is just too labile to be preserved under any natural circumstances, and the prevalence of recycling is essential for ecosystem function and maintenance. The true input term for marine sediments is the carbon delivery flux (CDF), i.e. the flux of carbon actually reaching the seafloor, which varies with water depth. Preservation is expressed by the burial efficiency (BE) – the percentage of the CDF that actually survives early diagenesis – which is indicated by the TOC becoming asymptotic (quasi constant) with depth, commonly at about 50 cm below the seafloor, as bacterial activity slows down. As for our purposes, TOC content is the ‘unknown’ property and the OCAR is derived from the product of the estimated CDF and BE (rather than by the conventional TOC%/100 x MSAR formula).

The general TOC equation makes it clear that there is no unique pathway responsible for organic-rich sediments. A high TOC content could reflect high productivity, unexceptional productivity combined with enhanced preservation, or unexceptional productivity and preservation combined with just low dilution by minerals, or indeed other combinations (and perhaps all scenarios – just in different places). The dominant term in the IPD equation will vary from one place to another (and through time), and no single explanation will apply universally. In any setting where one IPD term is effectively constant, the other two terms will become the main sources of variance. Only if two of the terms are almost constant will a single term be locally dominant. The observations that classic black shale source rocks are often condensed and exhibit geochemical, palaeoecological and sedimentological indications of dysoxia-anoxia imply that the combination of reduced dilution and elevated preservation is perhaps the most potent overall. The productivity required to produce oxygen depletion depends upon the circulation regime. If preservation is high and dilution is low, the productivity required to explain a specific TOC content is significantly reduced.

Model Description

To model TOC and HI, we need to know or at least estimate the primary productivity and water depth in order to calculate a CDF. We also need to understand variations in preservation in response to carbon flux, sedimentation rate and dissolved oxygen. These data are often not directly accessible from ancient sediments (or with the desirable accuracy), so we must turn to data from modern environments and sediments to help us understand and quantify these factors and their relationships. We can then apply this knowledge to ancient palaeogeographies by making the assumption that the fundamental relationships are relatively unchanged through geological time. Although many things may differ between the modern world and the past, we believe this approach has value and is capable of producing viable predictions given the overall levels of uncertainty.

The OFP Model utilises published equations for the key IPD relationships, plus a number of custom ones based on reanalysis of published marine sediment data. The model was developed with multiple options to accommodate a number of different potential scenarios. This is so it can be applied and calibrated to generate more precise regional predictions where the local conditions are better known, giving the model the potential to achieve much greater predictive power. It is therefore important to emphasise that the global TOC predictions delivered in Globe are intended only for providing a general appreciation of source rock presence and quality. Application at the global scale presumes that the algorithms utilised are equally valid everywhere, which is unlikely to be the case.

The relationships of the key variables were often harvested from data in multiple papers on different geographic areas and thus represent very generalised trends that might not necessarily apply well in a given specific area; conversely, some may be biased by data from a specific region. Use of global data invariably results in a larger error bar than if they had come from just one region where all factors would be expected to be more uniform. Obvious outliers were filtered to help remove noise. New data are constantly being produced and methodologies are revised, so no algorithms based on empirical relationships can ever be 'fixed in stone'.

In order to predict the TOC content or the HI, the model first simulates net primary productivity (NPP), which is based on latitude, water depth and distance from the coastline. Given productivity values, carbon fluxes (CDF) can then be estimated from the modelled water depth. The productivity values can also be substituted into Getech's custom equation for predicting background offshore sedimentation rate (LSARbkg), which is based on depth, productivity and distance from land. Sedimentation rates and carbon flux values allow us to estimate BE, and from the BE and CDF, we can then derive a marine organic carbon accumulation rate (MOCAR). Conversion of linear into mass sediment accumulation rates then provides us with everything we need to calculate location-specific TOC estimates using the basic (arithmetic) TOC equation. A schematic of the approach for marine TOC (MTOC) values is shown in Figure 1.

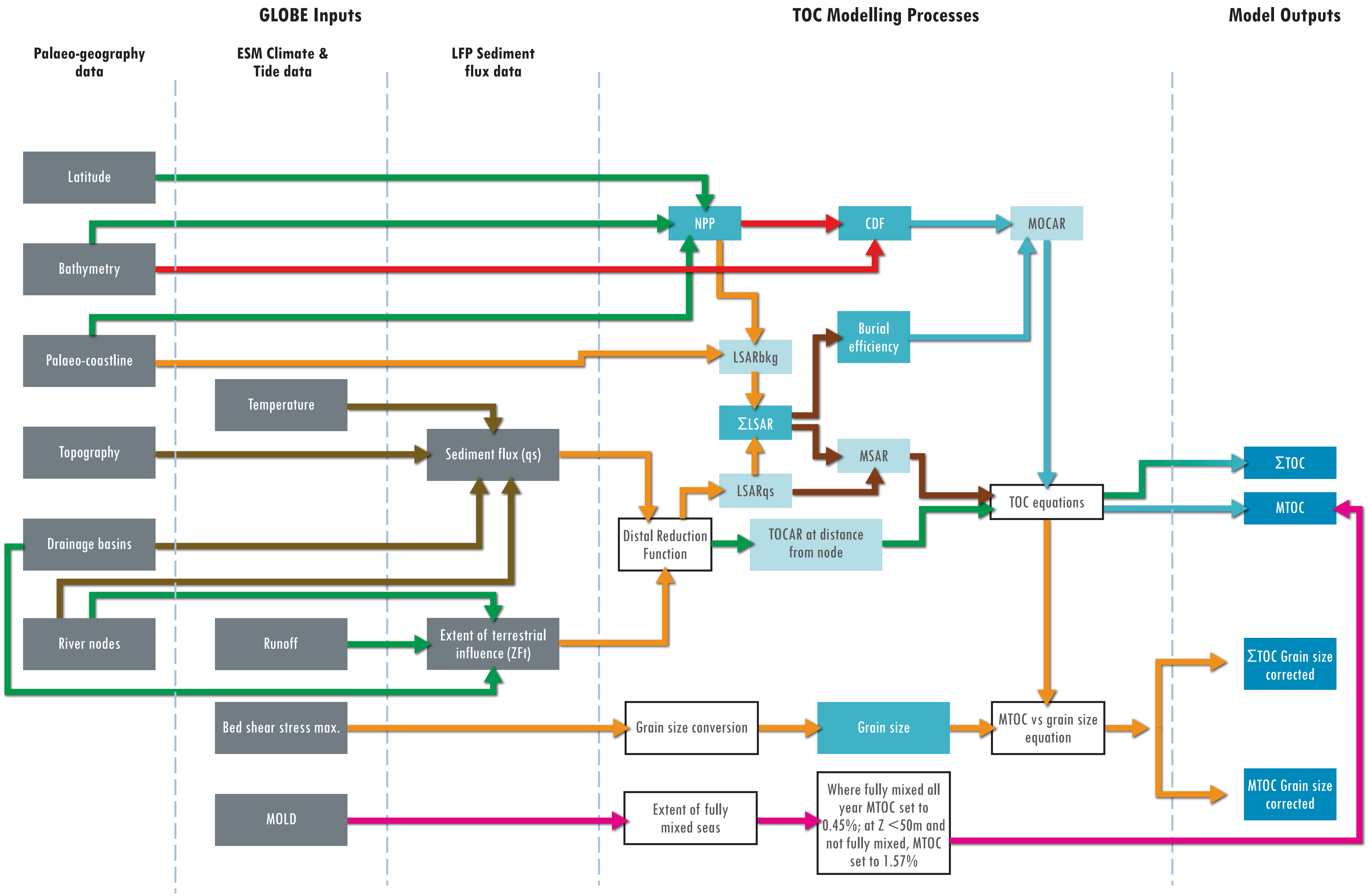

Figure 1: *A summary of the OFP model processes for calculating TOC.*

Some Limitations of OFP

OFP was developed with some intentional design constraints. Other constraints are imposed by the inherent limitations of equations or a lack of appropriate calibration data. Constraints include the following:

- The predicted TOC and HI values assume that the sediments are mudrocks (except in areas of high predicted tidal bed shear stress (BSS) and when tide model results are available).

- The predictions are for snapshots in time; they thus apply to beds rather than whole source rock formations (perhaps intervals of ~1,000 years – very much shorter timeframes than those of the stage-level maps used as the main input). Conditions will vary through time (e.g. through systems tracts or Milankovitch cycles) and assessing this would require multiple model runs with adjusted input values (plus an awareness of how the changes may be temporally correlated). The thickness of sediment with the predicted properties depends on how long the conditions represented by the modelled input values are thought to have persisted.

- OFP cannot currently model the essentially in situ production and accumulation of terrestrial OM (as in peats or coals).

- Lacustrine source rocks are not currently modelled.

- The OFP methodology cannot model sediments whose OM input is derived from benthic algal or microbial mats (some carbonate, sabkha and Precambrian facies).

Model Settings/Parameters

The OFP Model offers a large degree of choice in terms of its model settings to allow for the testing of various scenarios and to offer the flexibility for more constrained regional predictions to accompany regional studies and commissioned work. It is therefore necessary to determine the most suitable algorithms/equations and conversion factors to be applied for global predictions. The following sub-sections outline the general workflow for model runs and describe the application of the model to generate the OFP layers delivered in Globe.

Current OFP Model Workflow

The generic procedure is as follows:

1. Conduct a literature review to identify probable dissolved oxygen regime (not applicable for global predictions)

2. Gather relevant input data from Globe, i.e. palaeogeography map and corresponding digital elevation model (DEM), mixed ocean layer depths, maximum BSS, sediment flux and terrestrial influence dataSelect relevant NPP equation

3. Select an adjustment (%) if desired

4. Select a relevant CDF equation

5. Select a relevant LSARbkg equation

6. Decide whether to include fluvial linear sediment accumulation rate (LSAR; requires sediment flux and terrestrial influence data)
    a. Select summative or replacive model for LSARbkg and LSARqs integration
    b. Choose node overlap rule
    c. Select an adjustment (%) if desired

7. Decide whether to cap LSARbkg
    - Select a LSARbkg adjustment (%) if desired

8. Define the O2 versus water depth profile (not applicable for global predictions)
    - Decide whether to link upper transition to global circulation model (GCM) MOLD (if available)

9. Select a relevant BE equation (NB. Only some of them use O2)

10. Select the TOC type (MTOC, ΣTOC or direct TOC); ΣTOC only if a Globe Climate data is available
    a. If ΣTOC, set river node TTOC value
    b. Choose a method for TTOC attenuation

11. Choose the method for HI (HIA, MHI, ΣHI_Ftr or ΣHI_Fsi)
    a. If HIA, choose analogue HI vs. MTOC or enter custom equation
    b. If marine HI (MHI) or ΣHI, choose FS vs. HI relationship
    c. Adjust terrestrial HI (THI) end members if desired

12. Execute the program to generate the maps (TOC, TOCgsa, HI)
    - Grain size, NPP, CDF, LSAR and BE maps can also be generated to help with the evaluation of the TOC and HI maps

13. Examine the output, modify one or more settings, and re-run as required

Model Settings for Globe Data Layers

For the present set of global OFP maps, only specific settings were used (for simplicity or because some options are inappropriate for global maps). These settings are summarised below:

Workflow	Model Setting/Equation Applied	Notes
1. Literature review	Not pertinent for global predictions	Applying a single global oxygen profile is unrealistic and would produce unreliable results.
2. Input data	Data required: DEM, palaeocoastline, mixed ocean layer depths, maximum BSS, sediment flux and terrestrial influence data	Palaeogeography, GCM and tidal model outputs required for the model calculations.
3. NPP equation	Mirrored	Generalised trend with water depth, distance from land and latitude, based on the greater amount of modern sediment data from the northern hemisphere and then mirrored at the equator.
4. CDF equation	Pace et al. (1987)	The CDF equation that appears to work best overall in our appraisals.
5. LSARbkg equation	Getech custom	Uses depth, distance from land and the estimated palaeoproductivity (NPP); more realistic than depth only equations.
6. Inclusion of fluvial LSAR	Included for integrated marine and terrestrial TOC and HI predictions (ΣTOC and ΣHI). Node overlap rule applied.	Allows a simplified estimate of terrestrial OM supply and dilution effects adjacent to river mouths. Where river nodes overlap, the model uses the highest predicted fluvial LSAR value.
7. LSARbkg cap in shallow proximal settings	None applied	Effect appeared to be minor for global maps because it occurs primarily at depths of <50 m. It was thus omitted.
8. Oxygen profile set	Not applied, as no single profile is applicable globally. Mixed ocean layer data used to define fully/partly oxygenated zones to account for oxygen.	As a partial alternative, mixed ocean layer depth was used to define coastal areas where the water column is fully mixed all year. These are presumed to be fully oxygenated and thus to have poor preservation of marine OM (HI = 100 mgHC/gTOC, and thus a TOC of 0.45%).
9. BE equation	Betts & Holland (1991)	Assumes preservation is dependent upon LSAR only and does not require oxygen profile to be set.
10. TOC type	IPD model with fixed values for oxygenated zones and shallow waters of >50 m	Where depth is too shallow for a CDF equation to be valid, a constant is used based on the median modern TOC for marine sediments shallower than 50 m (1.57%). This value is treated as MTOC as the terrestrial fraction of the modern TOC is mostly unreported.
11. HI method	Derived from the predicted MTOC	Utilises a HI vs. TOC relationship based on selected modern-Holocene marine sediment data. For constant TOC values of 1.57%, this yields a HI of ~235 mgHC/gTOC .
•12. Results	• Grain size • NPP • CDF • LSAR • BE • MTOC and HI (two layers) • Integrated marine and terrestrial TOC and HI (two layers) • Grain size adjusted predictions for all TOC and HI data (four layers)	Grain size adjusted TOC and HI maps illustrate the possible effect of tides on the predicted values (but not other grain size effects).

Key OFP Parameters Delivered in Globe

Grain Size

The tidal BSS values are converted into an estimate of the maximum grain size that can be transported and thus also deposited (the so-called competent grain size); an example of these data is shown in Figure 2. The size is expressed in phi units (negative log base 2; with higher values being finer and lower values being coarser; phi = 0 corresponds to a diameter of 1 mm). The actual grain size may be equal to or less than the reported value, although finer-grained sediment would tend to be resuspended and deposited elsewhere during the highest energy phase of the tidal cycle. The parameter does not take into account 1) provenance effects that may limit the grain sizes potentially available, 2) areas of non-deposition or 3) wave, storm and gravity flow processes.

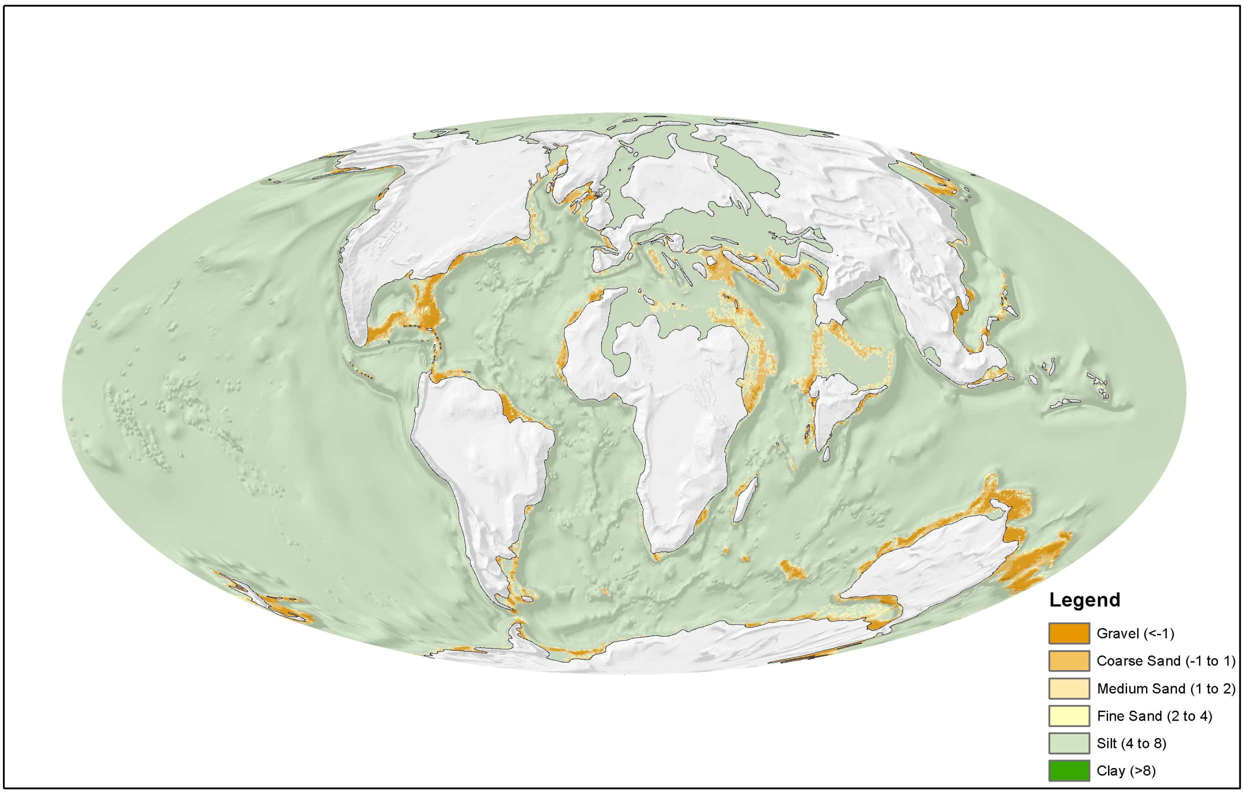

Figure 2: Example of the OFP model grain size parameter from the Ypresian.

The calculated phi values are based on fitting two polynomial regressions to the boundary ranges of BSS and to the equivalent grain size given in Berenbrock and Tranmer (2008). As these data are for a fluvial and confined flow regime, the relationship is probably not especially robust, but it helps to give an impression of real scale to the inferred maximum grain size.

For values of BSS of 0.0378–0.47 Nm-2, the regression (in Excel format) is:

mm = 0.0593-(1.7714*BSS)+(18.7109*BSS^2)-(22.7289*BSS^3) *Equation 3*

For values of BSS values greater than 0.47 Nm-2, the equation is:

mm = 0.8381+(1.2188*BSS)-(0.0007*BSS^2) *Equation 4*

These values were then converted to phi units by taking their Log10 values and multiplying by -3.3219.

For maximum BSS values of less than 0.0378 Nm-2, there are no data in Berenbrock and Tranmer (2008) to constrain the relationship with grain size, and extrapolation appears inadvisable owing to the evident non-linearity. The finest calculated phi grain size is 6.0 (15.6 μm, medium silt).

Net Primary Productivity (NPP)

Palaeoprimary productivity (PPP) is typically an unknown value for ancient sediments. Quantitative estimates of PPP require TOC values, sedimentation rates, sediment densities and porosities (and there are at least 10 different published equations). If these input data were all known, there would be no need for a TOC prediction. PPP calculations are not routine, and published examples come mostly from a small number of academic studies. In most cases, we need a different approach to PPP estimation.

The algorithm we use to derive the productivity estimate is based on a global map of the mean of 8 years of modern annual mean productivity values derived using the remote sensing carbon-based productivity model (CBPM; Westberry et al., 2008). This map was kindly supplied by Robert O'Malley (Oregon State University). The key advantages of the remote sensing data are the greater and more consistent temporal and spatial coverage compared to conventional shipboard measurements. The CBPM was adopted because it is considered to be the best model currently available (O'Malley, personal communication, 2012) and also because the overall range of values was found to be more comparable to measured values than those from the main (older) alternative model (the VGPM model of Behrenfeld and Falkowski, 1997). At least partly due to the better sampling, remote sensing values are typically greater than conventional shipboard measurements (daily rates that have been extrapolated to a whole year, with some allowance for seasonal variability, although the details of this step are seldom discussed).

Only the NPP data that matched sites from which other modern sediment calibration data were available were included in the analysis (to help ensure a more cohesive data set). These NPP values were then regressed with depth, distance from land and latitude to provide an algorithm that could be used with any palaeogeography and DEM. The NPP estimate does not explicitly taken into account local factors like GCM-based upwelling, stratification regime or river nutrients, but it does reproduce higher values at the coast and at the equator, with these values diminishing offshore and toward the poles. Although based on the Present Day, the globally generalised nature of the extracted trend means that it is less likely to be 'over-specified' (i.e. too strongly linked to specific modern features). An example of the modelled NPP results is shown in Figure 3.

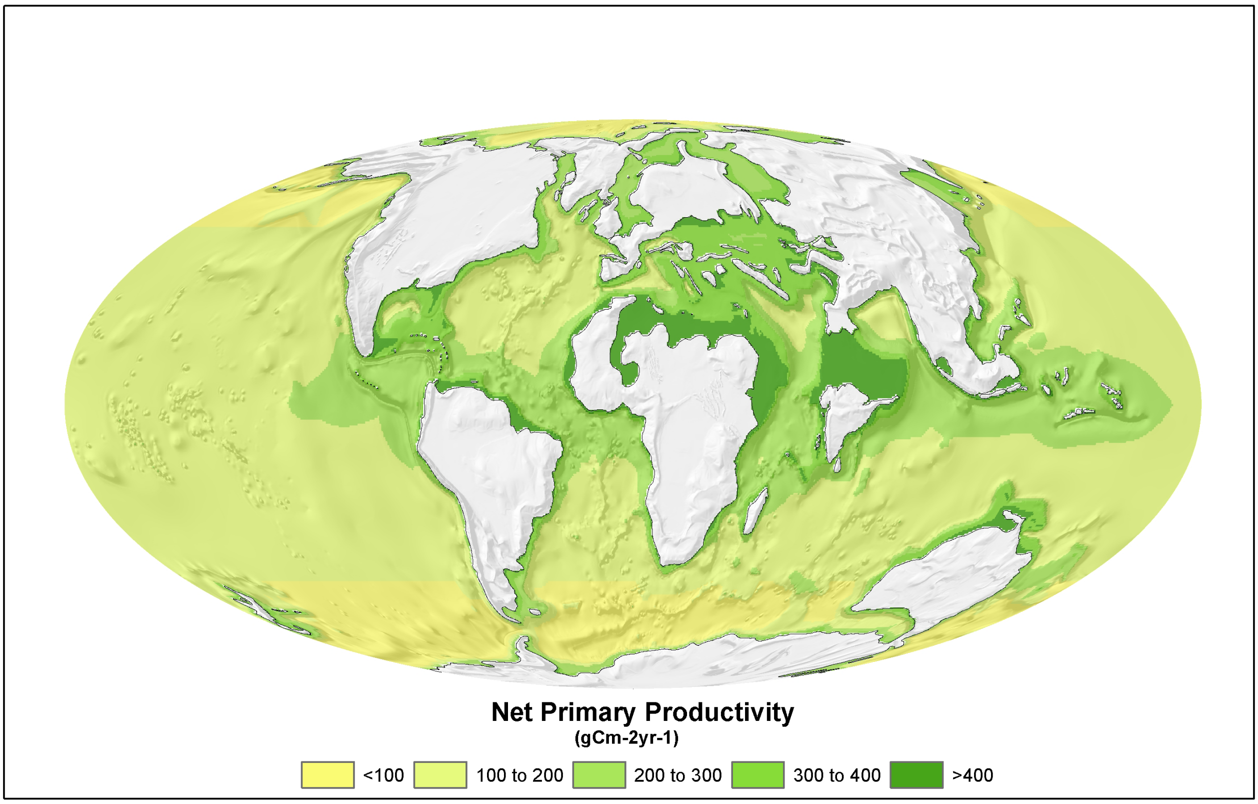

Figure 3: Example of the OFP model NPP parameter from the Ypresian.

The best regression results for the modern data were obtained by treating data from each hemisphere separately. The r2 value for the multiple regressions is only 0.6 for each hemisphere but given the reasonably large number of sites (600 for the southern hemisphere and >2,700 for the northern hemisphere), this is still significant. The standard error of the estimate (SEE) is about ±100 gCm-2 yr-1.

It was considered that modern hemisphere difference would be unlikely to remain constant through time due to changes in climate, ocean circulation and continental configuration. Furthermore, because there were more calibration data available for the northern hemisphere (sites there had TOC data as well as CBPM estimates of NPP), the northern hemisphere NPP trend was calculated and then simply mirrored about the equator.

The integrated northern hemisphere formula is:

((((501.9813+(-38.0398*LOG10(water depth))+(4.1074*0)+(-54.6658*LOG10(offshore distance)))- (637.273+(-101.215*LOG10 water depth))+(-2.685*0)+(-3.838*LOG10(offshore distance)))/2)+((((501.9813+(-38.0398*LOG10(water depth))+(4.1074*0)+(54.6658*LO G10(offshore distance)))-(637.273+(-101.215*LOG10(water depth))+(-2.685*0)+(-3.838* offshore distance)))/2)*-0.0111*latitude + 1))+637.273+(-101.215*LOG10(water depth))+(-2.685*latitude)+(-3.838*Log10(offshore distance)) *Equation 5*

Carbon Delivery Flux (CDF)

The OFP Model can calculate CDF using any of 22 equations (published or derivatives) based on water depth and NPP. When using the modern sediment equations for calibration purposes, the CDF values used were either ones based on near-bottom sediment trap data or calculated values where the CDF was reconstructed from the sum of the OCAR plus the carbon oxidised, where the latter was based on pore water and/or diagenetic modelling by the authors of the data set. Although OFP necessarily uses 'top-down' predictions of CDF (from NPP and water depth) in its ancient predictions, relevant OFP equations were calibrated using only documented 'bottom-up' CDF values as these are thought to be more reliable.

Top-down equations presume that the OM preserved in the sediment was supplied only vertically from waters where the NPP was estimated. This is a significant simplification as there are obviously also lateral fluxes due to currents, resuspension and nepheloid gravity flows (especially on the inner shelf and on topographic slopes) to consider. The magnitude of these lateral fluxes is very poorly constrained even at the Present Day (and, of course, OM is not a conservative property). Their omission is more pragmatic than scientific. The true CDF (bottom-up) is often likely to be higher than any top-down estimate, and the latter are thus relatively conservative estimates.

All published carbon flux equations, which are based primarily on open-ocean data, are not valid for depths of less than 100 m, and no equation is likely to be meaningful at depths of less than 50 m (where the formation or preservation of basinal source rock facies also becomes increasingly unlikely). To provide some estimate for palaeowater depths of between 50 and 100 m, we have improvised a separate equation based on Wassmann's (1990) equation for estimating carbon export below 50 m, plus a linear interpolation between this and the ordinary equation predicted flux for 100 m. At depths shallower than 50 m, the water column is likely to be fully mixed and unsuitable for source rock deposition, and any organic-rich sediment deposited is less likely to survive subsequent erosion.

For global predictions, the CDF equation is based on that of Pace et al. (1987):

Equation 6a (Pace et al., 1987) = depths ≥100 m

CDF1a = 3.523*((NPP)^1)/(Water depth ^0.734) *Equation 6a*

Equation 6b (Pace et al., 1987; Wassmann, 1990) = depths 50–99.9 m

CDF1b = (0.049*(NPP^1.41))-(((0.049*(NPP^1.41))-(3.523*((NPP)^1)/(100 ^0.734)))/50)*(Depth-50) *Equation 6b*

These have been utilised as they have been successfully applied to modern studies of both oxic ocean waters and the anoxic Cariaco Basin (Thunnell et al., 2000). We have found that it provides a conservative estimate of CDF, but one that has an above-average performance at shelf depths and has a better agreement with measured (bottom-up) CDF values. An example of the modelled CDF results is shown in Figure 4.

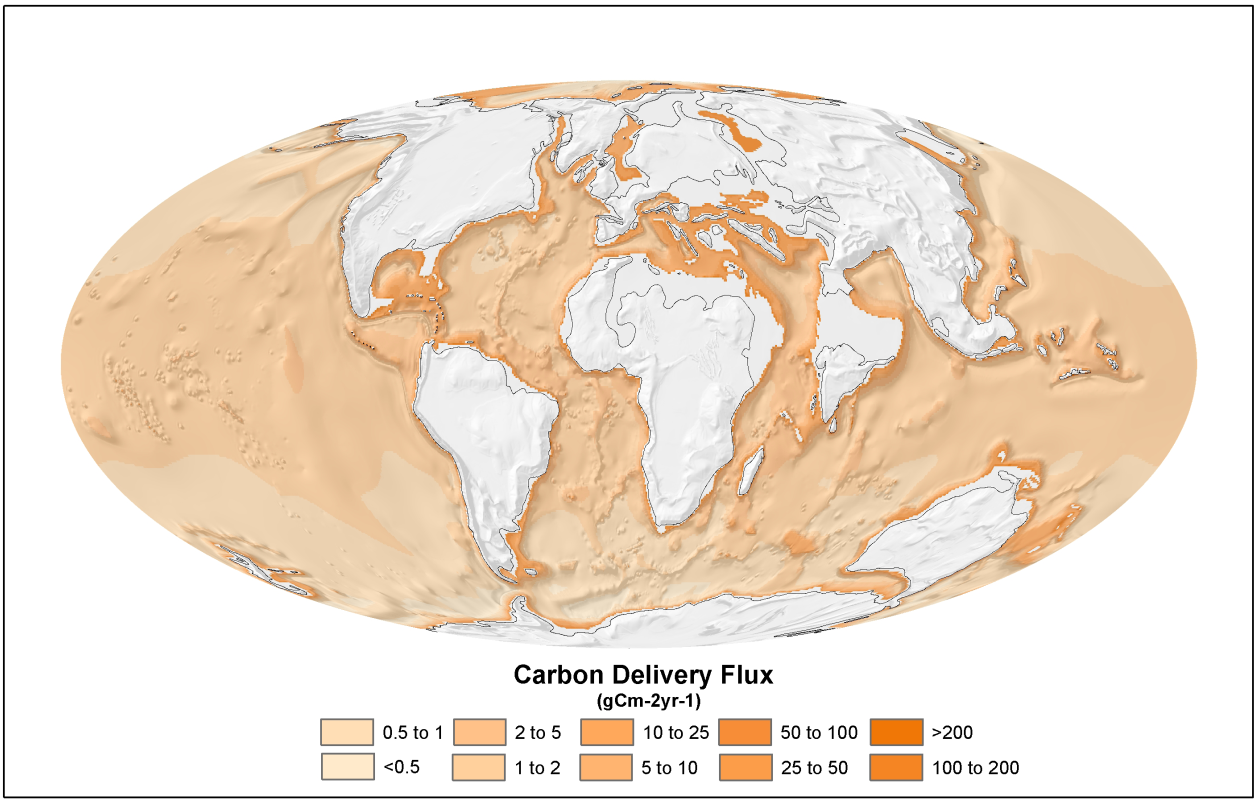

Figure 4: Example of the OFP model CDF parameter from the Ypresian.

Linear Sediment Accumulation Rate (LSAR)

Sedimentation rates are crucial for assessing BE in oxic facies and dilution in all facies. The linear rates (thickness/time) can be converted into mass sediment accumulation rates (MSAR) using a user-defined density and porosity or determined from linear (or multiple) regression of modern LSAR and MSAR. The regression approach is useful because the OM component within the MSAR can be removed and omfMSAR can be predicted from LSAR.

All sedimentation rates used in modelling TOC are short-terms ones (mostly expressed in cm/ka). This is because these are the rates relevant to the duration of the processes that influence the production, deposition and preservation of OM. The TOC content of immature sediments is 'locked in' relatively soon after burial. Although longer term (geological) rates might be important for preserved total thicknesses, they are not what control the TOC content.

OFP splits sedimentation rates into two components: the background (LSARbkg) and local fluvial LSARqs related to sediment discharge from river nodes (the latter is calculated in the sediment flux modelling stage; see the separate Sediment Flux User Guide for further details).

LSARbkg

The LSARbkg is not just a biogenic pelagic rate, but the mean sedimentation rate for any sediment that is not related to a specific fluviodeltaic point source (river mouth).

This estimate of LSAR is based upon a multiple linear regression analysis of published modern marine sediment data. Being based on modern sediments, these are short-term values and essentially uncompacted, but these are the rates that are most relevant to the short-term processes that influence OM deposition and preservation. They will overestimate the long-term sediment accumulation rate.

The equation used is as follows (in Excel notation):

LSARbkg = (10^(1.5808+(-0.435*LOG10(water depth)+(0.4413*LOG10(NPP))+(0.621*LOG10(offshore distance))))*1.986 *Equation 7*

where offshore distance is in decimal degrees. The r2 value is 0.62, excluding outliers (n = 355). The last value in this equation (1.986) is a calculated statistical correction factor to correct the bias introduced by back conversion from log10 values (and without which the value appears too low compared to other depth-only predictions).

LSARqs

The combination of the Getech drainage modelling, climate model results and sediment flux modelling based on the Syvitski ART model (Syvitski et al., 2003) allows us to estimate the sediment discharge from each river node (Qs, in MT/a); further information on these methods is provided in the separate Sediment Flux User Guide. With some admittedly simplistic pragmatic assumptions, these data can be converted into distance-varying estimates of linear and mass sedimentation rates (LSARqs and MSARqs) of fluvially derived sediment. The LSARqs is only calculated for areas within a radial distance of river mouths and is derived using a proxy based on the relationship between river discharge and the distance offshore at which modern δ13C values indicate the fraction of terrestrial OM falls to zero (ZFt); this is used as a proxy for the extent of terrestrial influence.

To convert sediment discharge (Qs) into an estimated sedimentation rate (LSARqs), we have to know the area over which the annual mass of sediment coming from the node is deposited. The indirect proxy we use for this is the ZFt radial distance, which is estimated using a Schultz and Calder (1976) type equation, then edited, supplemented and modified to extend it to a greater range of discharge without it reaching a premature asymptotic maximum. This equation links the ZFt to river water discharge (Q), and thus the terrestrial influence of larger rivers extends further offshore than smaller ones (to a maximum of about 300 km based on the Amazon profile perpendicular to the coast). Further details of how ZFt is calculated can be found in the separate Sediment Flux User Guide.

A 3D geometry must be assigned to the sediment body deposited within the ZFt in order to relate the mass and area to a volume and thus thickness (via user-defined assumed density and porosity values). It is assumed that the debouching annual fluvial sediment load forms a semi-conical 180° fan, especially over extended periods of time (due to distributary switching, changing coastal morphology, etc.). This is unquestionably a naive representation of a prodelta but it has the practical advantage that it is relatively easy to both calculate and apply universally. Although an elongation of fluvial lobes due to alongshore drift is easily envisaged and the direction is apparent from the Climate model ocean current direction, the modelling of the changing depositional geometry of the resulting sediment body would be challenging (and the effort perhaps not justified considering other uncertainties).

Using basic conical geometry, we can determine the height of the apex of the sediment cone with twice the fluvial sediment (half cone) volume, which will be equivalent to the annual sediment increment at the node (cm/a). We not only need the height of the apex of the cone, but to calculate this correctly, we also need the volume of the full cone. The LSARqs is then assumed to decrease offshore radially and linearly with distance from its maximum at the apex of the cone (the node) to its minimum (zero) at the ZFt distance (as implicit in the conical geometry), where only the background LSAR is recorded (Figure 5). For simplicity, all nodes are currently handled identically.

Observed local short-term delta front/pro-delta sedimentation rates can be extremely high; modern examples range from about 4 cm/a (for the Fly River) to 10 cm/a (for the Amazon) and up to 35 cm/a (for the Rhône). Such rates are not geologically sustainable, and longer-term rates will be reduced because of discontinuities in deposition and intervals of erosion. Consequently, after the initial cm/a value is multiplied by 1,000 to convert it to cm/ka, an adjustable constant stratigraphic completeness value (for ka resolution) is also applied, with the adopted default being the 48% cited for the Amazon by Sommerfield (2006).

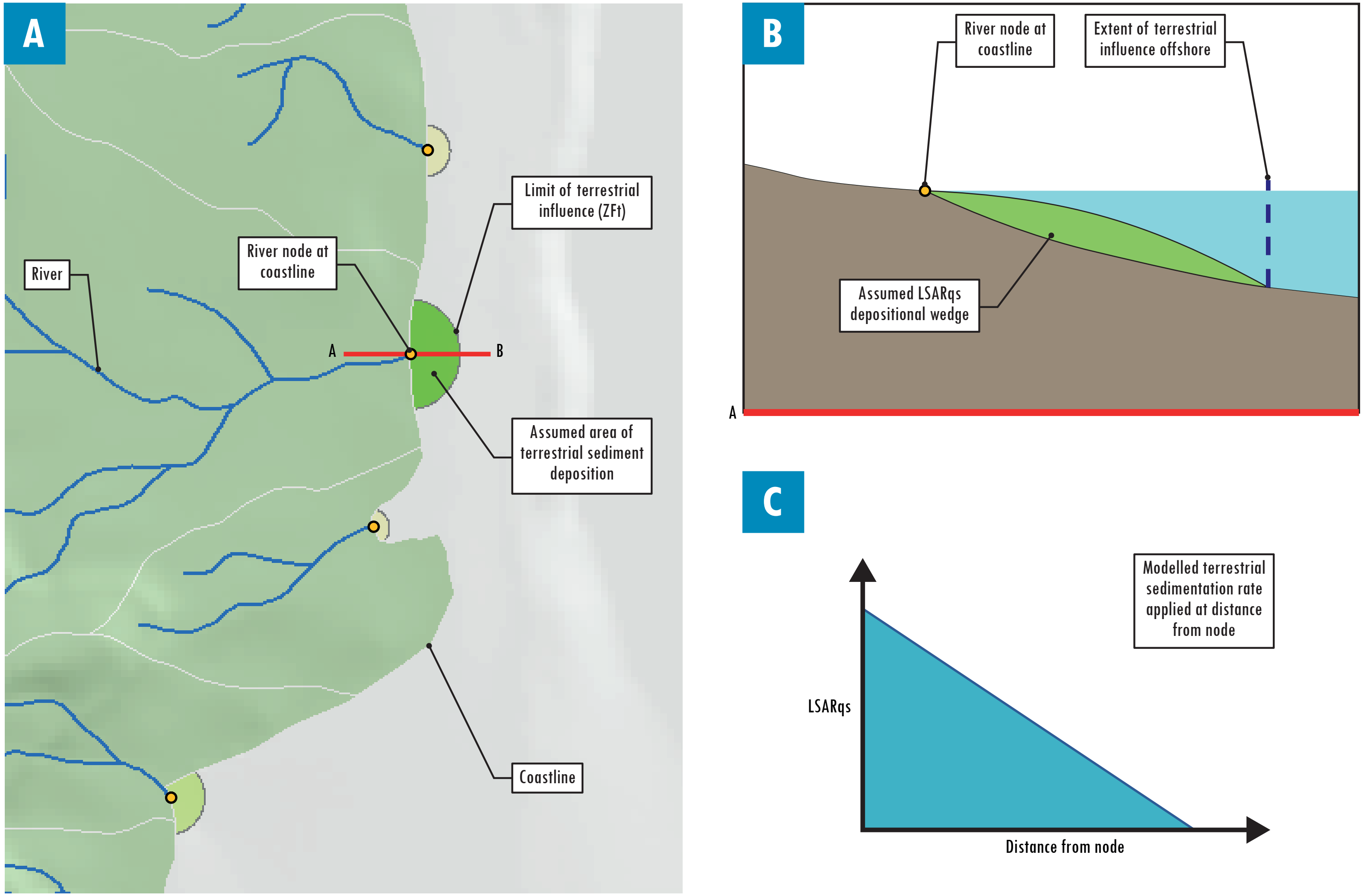

Figure 5: *A) Map view showing the extent of terrestrial influence (ZFt) and the area of terrestrial sedimentation assumed by the OFP Model. B) A schematic cross-section of the map view, demonstrating the assumed terrestrial sediment depositional wedge from the river node at the coastline to the limit of terrestrial influence (ZFt). C) A schematic representation of how the terrestrial sedimentation rate (LSARqs) is reduced by the OFP Model based on distance from the river node.*

Integration of LSARbkg and LSARqs (∑LSAR)

For the default LSARbkg equation, the distance used is distance from coast (Dc in degrees). For the fluvial sedimentation rates, the distance used is that from the river node (Dn in km). Within the ZFt radius, the Dn and Dc thus need to be known for each grid point, but only the Dc offshore of the ZFt. Within the ZFt radius, the LSARbkg and LSARqs could be considered to combine in either a summative fashion (both present and summed) or a replacive one (the background is entirely replaced by LSARqs at Dn < ZFt if the LSARqs is greater than the background), as represented in Figure 6. A replacive model has been utilised for the global OFP maps.

The ZFt decreases with discharge, and thus for smaller rivers fewer grid points, it will be incorporated within its radius. Much of the variation in LSARqs may also occur at a scale smaller than the grid size (~55 km at 0.5° x 0.5°), particularly for smaller rivers, so the overall impact on the maps will vary with the proximity of the coastline to the centre of the grid cell. Small rivers always dominate on a global scale, and as their ZFt is generally only about 40 km or less (i.e. below the grid cell spacing), the ZFt radius of many such rivers may not be expressed on the maps at all (e.g. up to ~45% of all the nodes for the Maastrichtian).

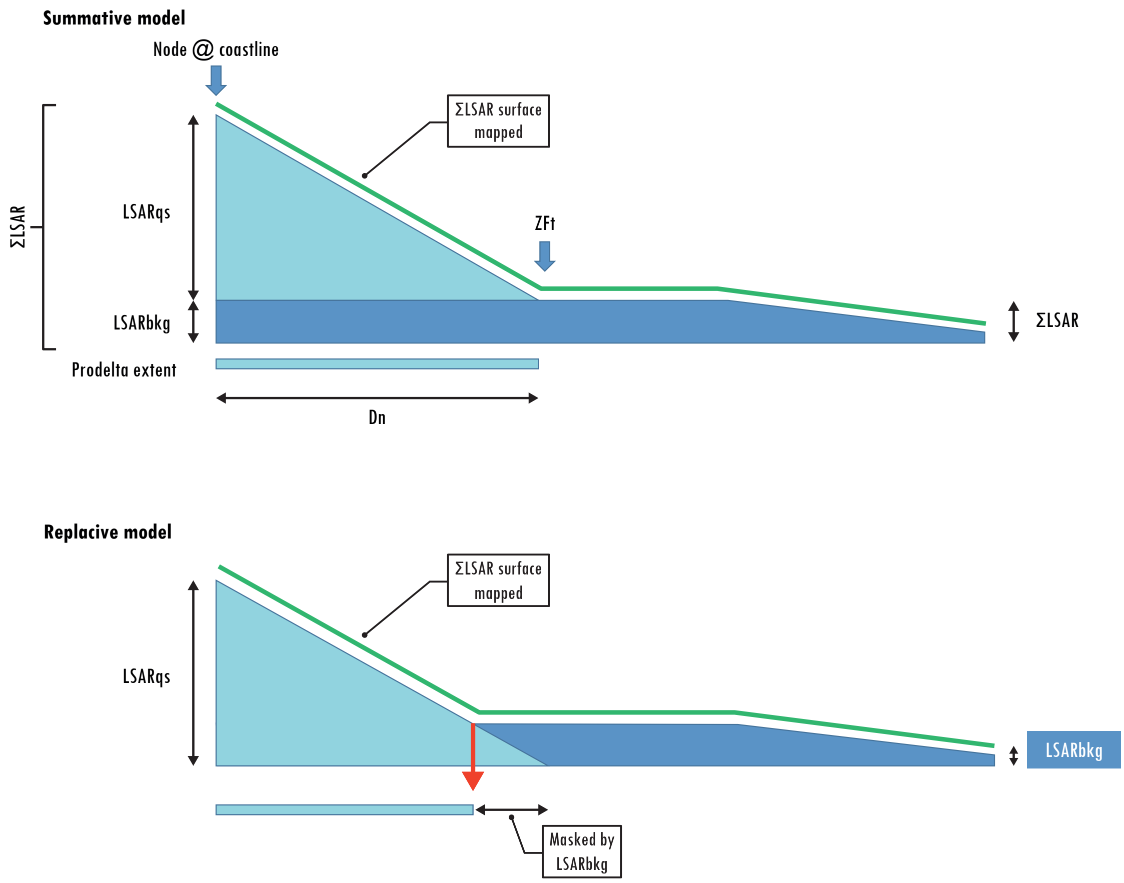

Figure 6: A schematic representation of how the LSARqs and LSARbkg can be combined, with the replacive model being applied for global LSAR data.

Burial Efficiency (BE)

BE is the OCAR divided by the CDF, expressed as a percentage. This is the fraction of the carbon flux that survives early diagenesis to be preserved in the sediment (generally at burial depths of 50–100 cm). There may be subsequent slow degradation with further burial, but the rates are low and the diagenetic signal will become smaller than that associated with changes through time. It has been found that this parameter covaries with sedimentation rate (Henrichs & Reeburgh, 1987), although it may also be influenced by other variables, including carbon flux and oxygen regime (Tyson, 2001), and thus oxygen exposure time (Hartnett et al., 1998).

Here, we have used the Betts and Holland (1991) equation for BE (Equation 8), principally due to it not requiring a defined oxygen profile.

BE% = (10^((1.39*LOG10(LSAR))/LOG10(LSAR+7.9)+0.34)) *Equation 8*

The BE increases with LSAR, but according to this equation, it has an in-built asymptotic maximum of around 54%, with BE flattening out above ~10 cm kyr-1. Once the BE attains its effective maximum (according to this equation), further increase in sedimentation rate will result in increasing dilution of the TOC (Tyson, 2001). An example of the predicted BE is shown in Figure 7.

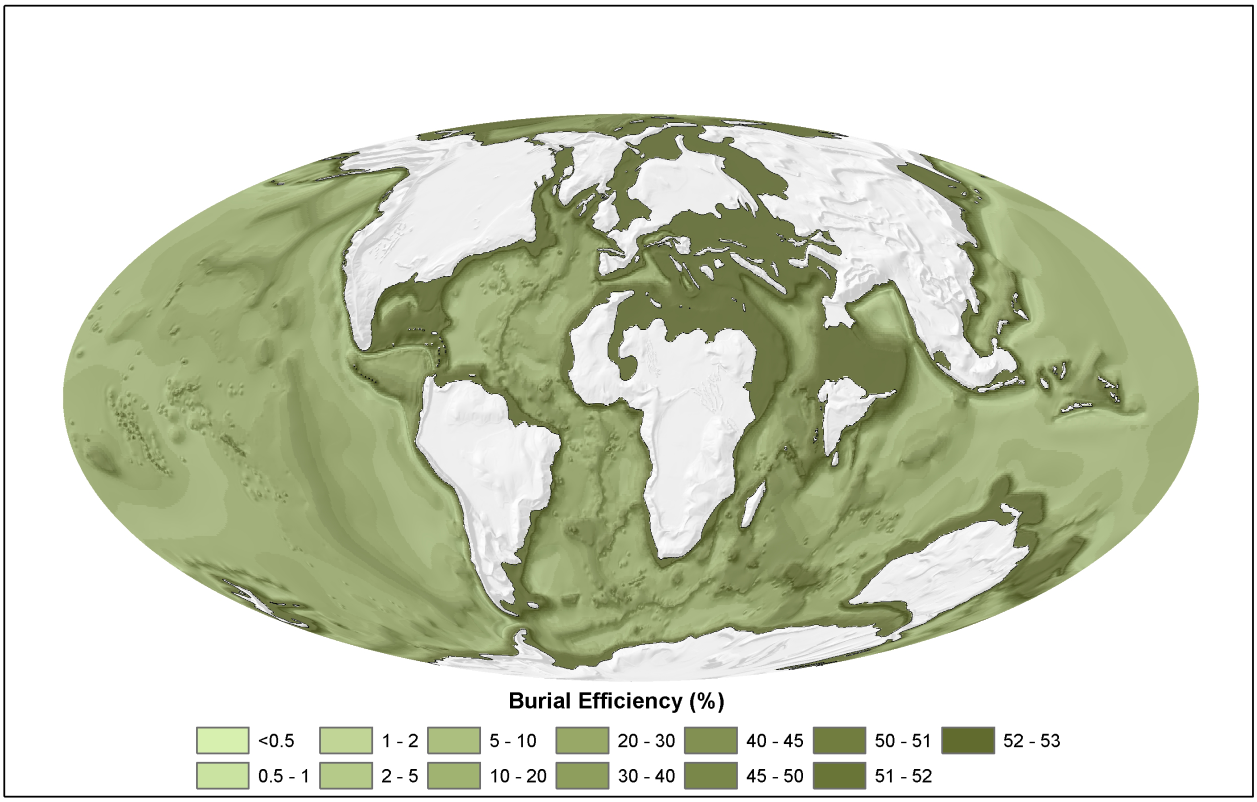

Figure 7: An example of OFP modelled BE from the Ypresian.

Total Organic Carbon (TOC)

Marine TOC (MTOC)

This is the TOC calculated using the fundamental IPD equation (Tyson, 2005):

$$TOC = ((Input \times Preservation) / (Input \times Preservation \times OMF) + Mineral\ Dilution) \times 100$$
Equation 9

where OMF is the conversion from TOC to OM (1.8 is used here).

In terms of the preceding parameters, the actual equation (in Excel format) is:

MTOC% = (((CDF * (BE%/100)) / ((CDF * (BE%/100)) * 1.8) + omfMSAR)) * 100 *Equation 10*

If the delivery flux and sedimentation rate are completely unconstrained by any actual known values (as here), one should not expect this equation to necessarily produce a close simulation of reality. It is important to emphasise that the calculated value is not our best guess of what the true TOC might be, but rather just the value one gets if one assumes the sedimentation rate, water depth, productivity and specific equations used above. The result may or may not be a good estimate of reality, and how well the equation performs will certainly vary spatially. In some cases, the pattern of relative variation may be more meaningful than the actual magnitudes of the calculated values. An example of the predicted TOC for the Ypresian is shown in Figure 8.

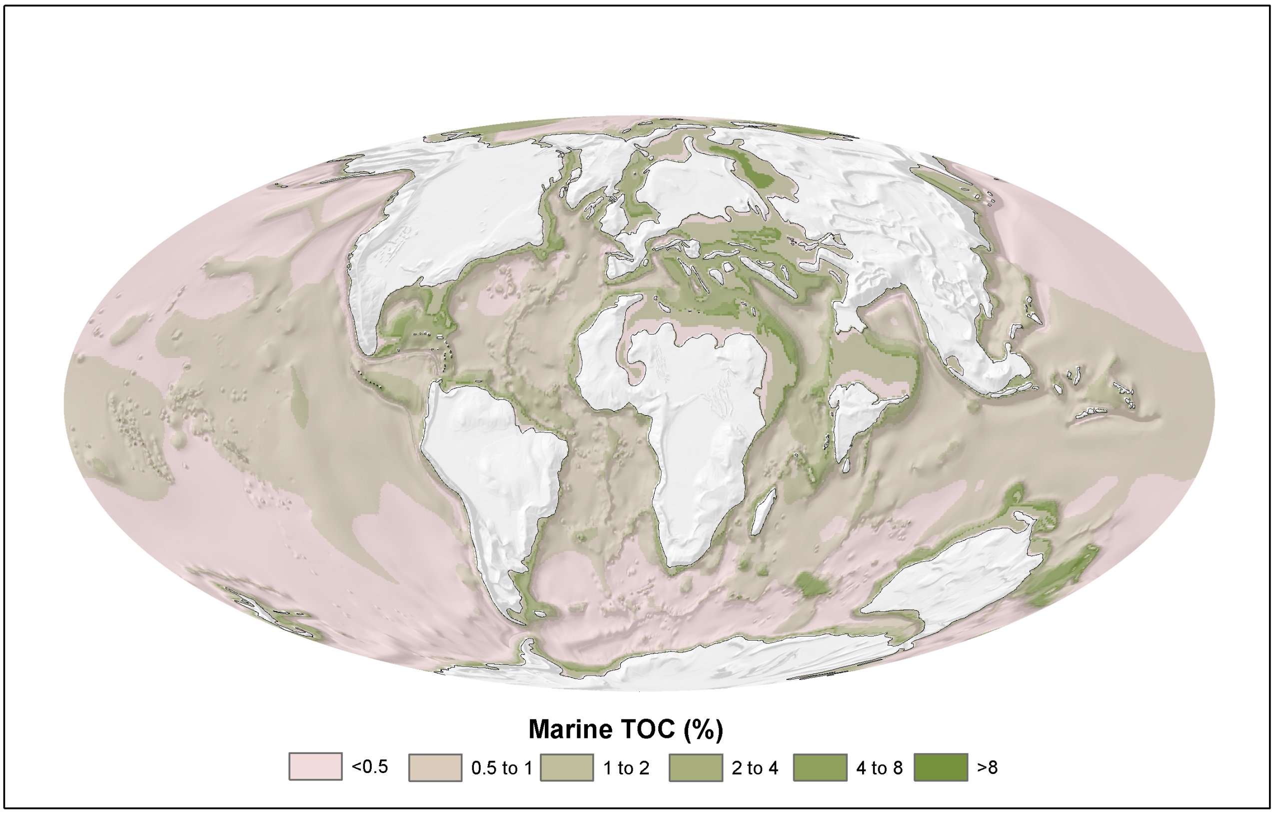

Figure 8: An example of OFP modelled MTOC from the Ypresian.

As the MTOC equation above requires an estimate of the CDF, which is not possible when water depth is less than 50 m, a different approach is required to avoid large areas of the shelf on the maps remaining blank. For most of these shallow-water areas, we have utilised the median TOC value of modern marine sediments based on a database of published values (1.57%, n = 1,846). However, where the monthly variation in the ocean mixed layer depth indicated that the coastal water column was continuously mixed and fully oxygenated all year, we have presumed that the marine OM would be degraded, resulting in an MHI of 100 mgHC/gTOC; the corresponding MTOC, based on the HI vs. TOC relationship utilised for estimating HI from TOC (see below), is 0.45%. In the coastal areas, additional spatial variation in the ΣTOC values (marine plus terrestrial TOC) results from the addition of terrestrial carbon and variable siliciclastic dilution.

Using the constant MTOC value of 1.57% for much of the shallow shelf means that there is often an unrealistically abrupt change in the ΣTOC values at the 50 m isobath (especially as the CDF into 50–100 m depth range may be an overestimate). It does, however, ensure that the oxic coastal facies are shown as having a lower quality organic facies.

Terrestrial TOC (TTOC)

Despite the additional flux of terrestrial OM from rivers, TOC values are rarely more than 2–3% in most prodelta muds (for samples unbiased by macroscopic plant debris). For simplicity, we assume that at the river node the terrestrial fraction (Ft) is 100%, and thus that the TOC here represents just TTOC. We also assume that the TTOC has a value of 3% at all river nodes. The TTOC is multiplied by the MSARqs value (derived from the fluvial Qs) to give the terrestrial organic carbon accumulation rate (TOCAR) at the river node. As the sedimentation rate (MSARqs) decreases with distance from the river node, the TOCAR thus also decreases proportionately. The TTOC can be calculated from the TOCAR and the MOCAR and omfMSAR values (and the OM factor); it varies from 3% at the river node to zero at or beyond the ZFt distance. Redeposition beyond the Zft, including that achieved by gravity currents, storms and alongshore drift, is not taken into account.

Marine and Terrestrial TOC (∑TOC)

The final mapped TOC values represent the ΣTOC, which is the sum of the MTOC and TTOC. At depths greater than 50 m and beyond the ZFt radius, the ΣTOC corresponds to the MTOC, but within the ZFt radius, it is a mixture of marine and terrestrial carbon. An example of the predicted summed TOC for the Ypresian is shown in Figure 9.

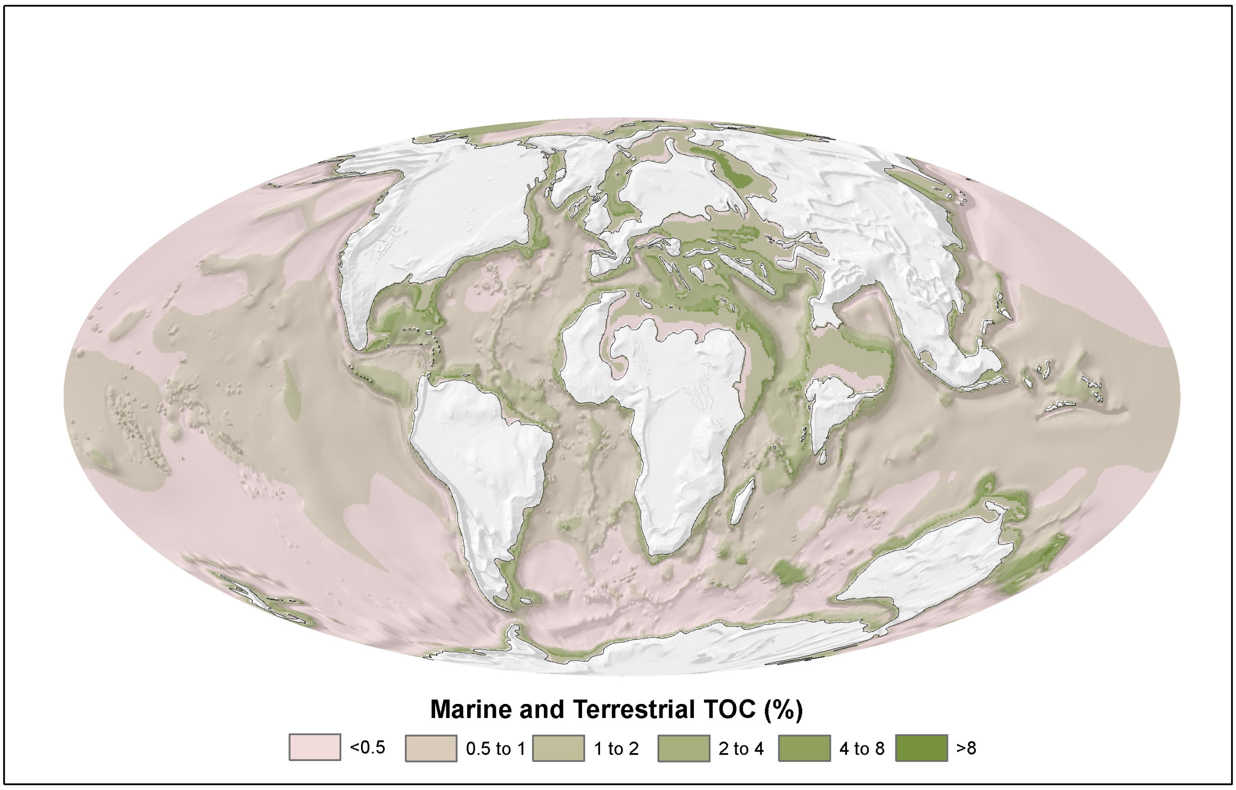

Figure 9: *An example of integrated marine and terrestrial TOC from the Ypresian.*

Hydrogen Index (HI)

Marine HI by Modern Analogue (MHI)

The HI of marine sediments is a function of the sources of the OM, the ratios in which they occur and their preservation state. The preservation state is primarily controlled by the dissolved oxygen/redox regime of the sediments. For regional applications, OFP can employ a posited dissolved oxygen versus water depth profile for use in predicting the MTOC and MHI distribution, but no single profile will be valid on a global scale. Consequently, the global OFP maps for MHI are instead based on an assumed relation between MHI and MTOC. In regional studies, we can utilise a HI vs. TOC relationship derived from observed data in turn derived from an analogue source rock facies, but for the global maps, we have used a relationship derived from modern to Holocene sediment data (although there are much less data available for this time period than there are available for ancient sediments). An example of the predicted MHI for the Ypresian is shown in Figure 10.

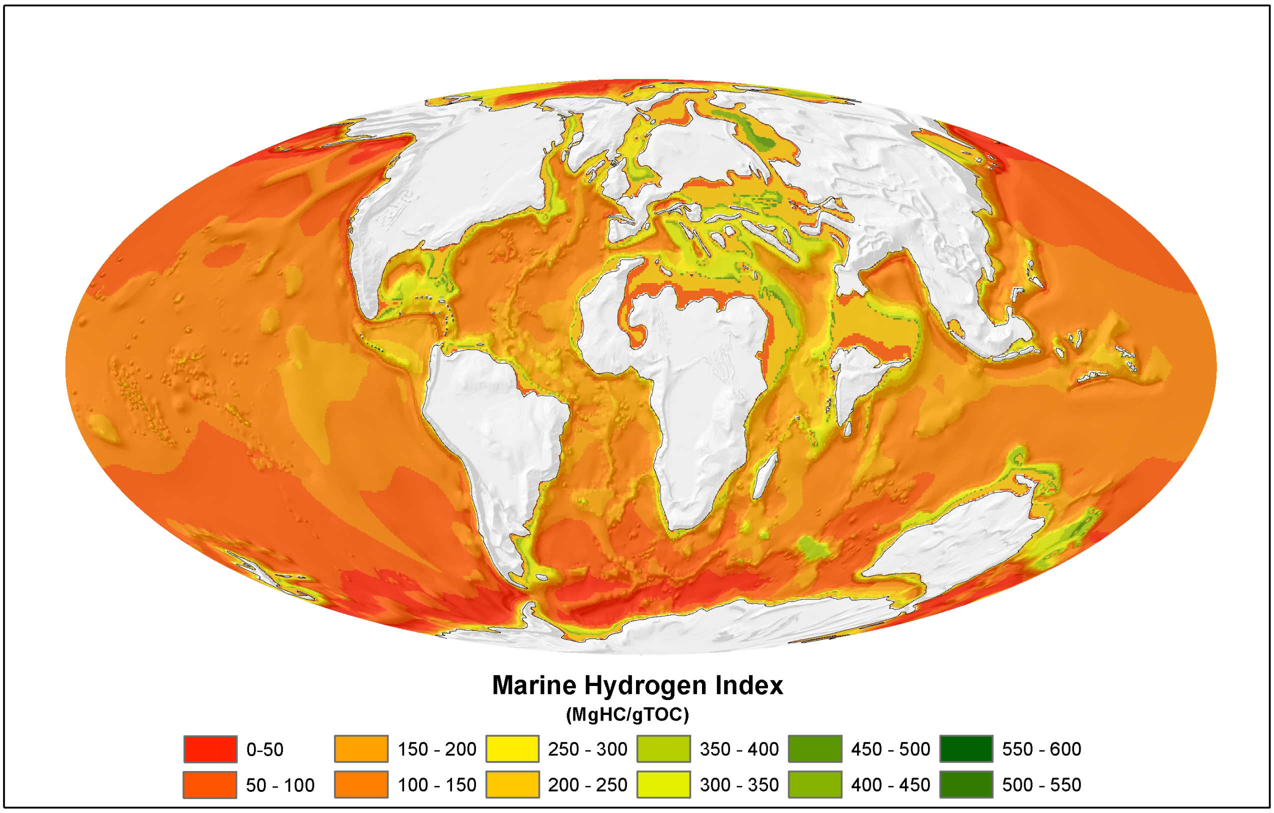

Figure 10: An example of OFP modelled MHI from the Ypresian.

Higher modern TOC values are associated with shelf to slope water depths and areas of higher productivity and/or lower dissolved oxygen, and these are also often associated with higher HIs. There is significant scatter in the TOC vs. HI data, but we know that theoretically the HI should show a positive and inherently asymptotic natural logarithmic (LN) relationship with TOC. Data that fitted this expected pattern were thus selected for regression. Three sets of data were utilised: modern upwelling/oxygen minimum zone sites from a composite marine sediment database (n = 166), data from the Benguela upwelling zone (Blanke, 2004; n = 28) and data from the Black Sea (Arthur & Sageman, 2005; n = 22). The three logarithmic best fit equations derived from each data set were then averaged to produce a single equation (in Excel format):

MHI = 107.02*LN(TOC)+185.79 *Equation 11*

where TOC is either the MTOC value from the IPD equation (depths of 50 m or more) or either of the two MTOC constants (0.45% or 1.57%) used where water depth is less than 50 m. The minimum permissible MHI value is set to 50 mgHC/gTOC.

Terrestrial HI (THI)

We modelled lateral variation in terrestrial HI (THI) using a simple distance-based linear mixing model. This is guided by the observations that normal coal vitrinite commonly has a HI of around 200 mgHC/gTOC, whereas dispersed marine phytoclast populations are more typically associated with an HI of about 100 mgHC/gTOC. Inertinite (Type IV kerogen) is generally considered to have a HI of about 50 mgHC/gTOC, and the fraction of inertinitic phytoclasts tends to increase distally due to selective preservation or transportation, regardless of the basinal redox regime (although based on phytoclast colour, it seldom seems to become dominant, except perhaps when oxygen exposure time is very high). Given the default two end-member values, the default distance-based mixing model produces a range in the THI of ~200 mgHC/gTOC at the river node to ~100 mgHC/gTOC at the ZFt (the seaward limit of terrestrial influence).

Mixing of Terrestrial and Marine HI: ∑HI

The global HI maps are ΣHI maps, an example of which is shown in Figure 11. At any given location, the combination of the terrestrial and marine HI, or ΣHI, is calculated from the sum of the MTOC fraction multiplied by the MHI and the TTOC fraction multiplied by the THI. The marine and terrestrial OM fractions are calculated from marine and terrestrial OCAR values (TOCAR and MOCAR, together = ΣOCAR).

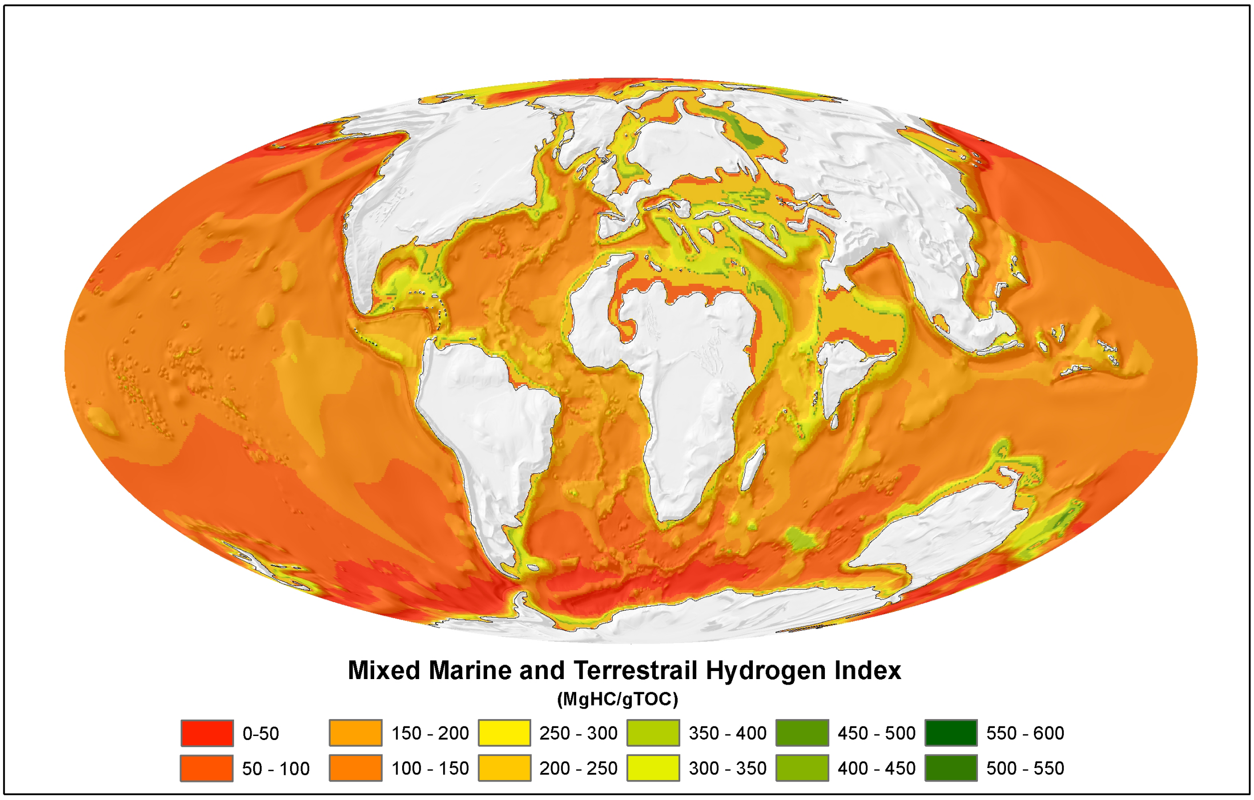

Figure 11: An example of integrated marine and terrestrial HI from the Ypresian.

Significant mixing of terrestrial and marine OM is generally a relatively localised and proximal effect; therefore, it is applied only adjacent to river nodes within the ZFt radius. Note also that, because the absolute THI value is often much lower than the MHI of well-preserved marine OM, the overall impact of the mixing effect on ∑HI is diminished in high MTOC facies. Where marine OM is poorly preserved, the MHI and THI values also converge.

Grain Size Adjusted ∑TOC and ∑HI

The modern sediment database used to derive the various equations used in OFP usually lacks information on the grain size. We have therefore assumed that the IPD-predicted MTOC values are for sediments whose modal grain size is equivalent to an 85% mud-sized content. Where the tide-predicted grain size (mud content) is lower than this, the TOC is expected to decrease because of a combination of hydraulic equivalence, surface area/volume, benthic reworking and winnowing effects. As noted in the Grain Size Section, the tidal model results have been used to predict the maximum or competent grain size that can be mobilised by the tides. These data can be utilised to adjust the TOC and HI values in the model according to the competent grain size predicted by the tidal BSS.

The tide-predicted phi grain size value is converted to an estimate of the mud content (%) using a regression of modern marine sediment data for phi values of 6 to 1.48 (medium-grained silt to medium-grained sand):

% mud = 13.065*(mean phi <=6) - 19.328 (r2 = 0.94) *Equation 12*

The degree of relative reduction in MTOC is estimated by using a documented relationship between mud content and TOC content (Diester-Hass & Muller, 1979):

%MTOC = (0.0257*%mud +0.1583) (r2 = 0.87, n = 44) *Equation 13*

If the calculated maximum phi grain size is greater than (finer than) 6.00, no MTOC adjustment is applied. Where the calculated maximum phi grain size is less than (coarser than) 1.48 (medium-grained sand), the MTOC is set to zero. For values in between, the percent TOC is adjusted according to the above equation. The adjustment in TOC (and thus HI) values can only be downward (reduced). TTOC values are not grain size adjusted because terrestrial OM has a different relationship to grain size.

Because the MHI values are here estimated from the MTOC, any reduction in MTOC will also decrease the MHI and thus the ΣHI. It is suggested that the global grain size adjusted ΣTOC and ΣHI maps should be compared to the unadjusted maps to identify areas where enhanced tidal mixing may have a negative effect on source rock quality. An example of such a comparison is shown below in Figure 12.

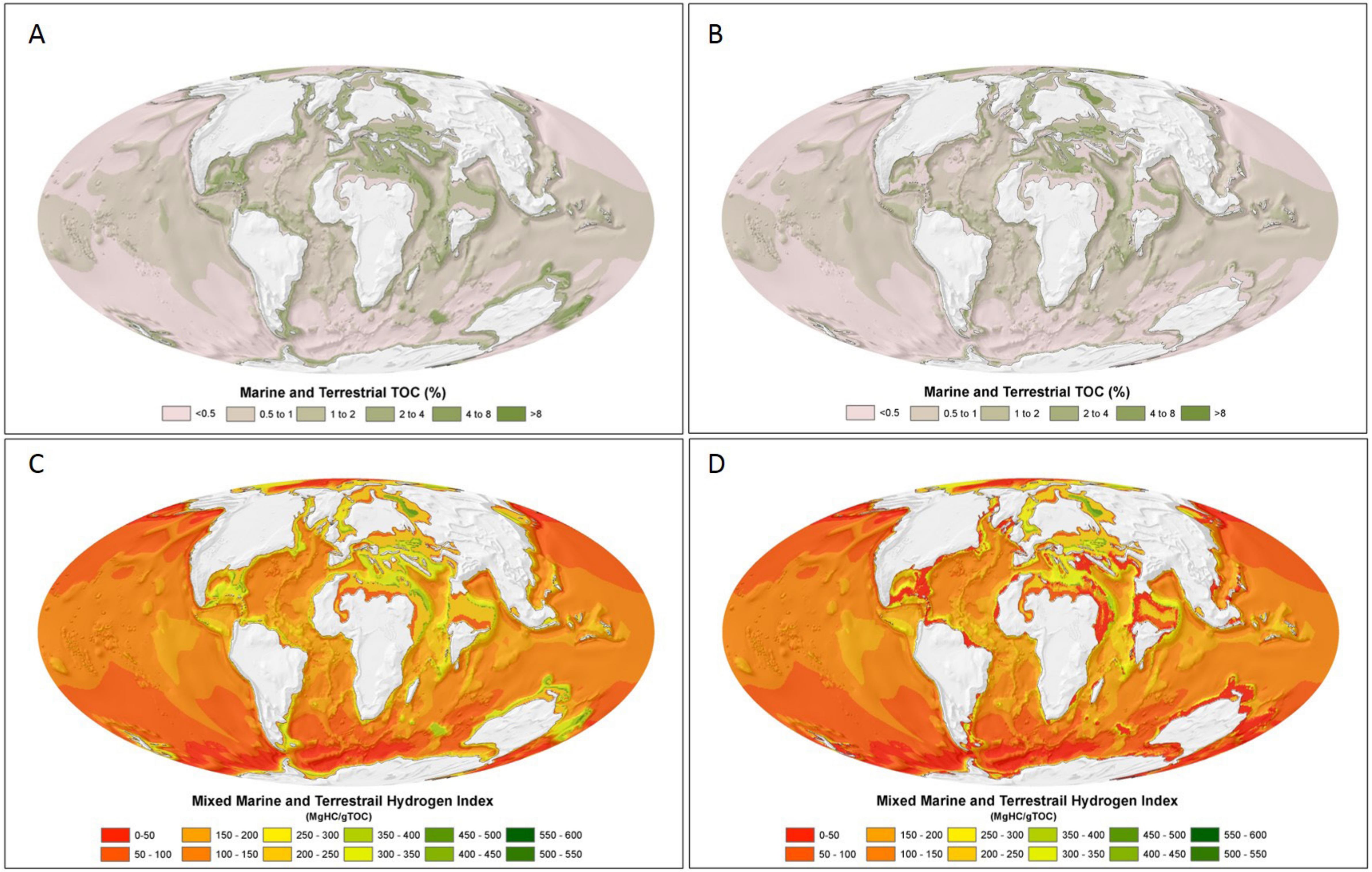

Figure 12: *A) OFP modelled summed marine and terrestrial TOC. B) OFP modelled summed marine and terrestrial TOC with grain size adjustment, showing a reduction in predicted TOC where a coarser grain size is predicted. C) OFP modelled summed marine and terrestrial HI. D) OFP modelled summed marine and terrestrial HI with grain size adjustment, showing a reduction in predicted HI where a coarser grain size is predicted. All examples are from the Ypresian.*

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