

Supporting documentation for data resource Sedimentary_OC_Quality_Reactivity.csv

Project	Sources, Sinks and Subsidies: Understanding Sedimentary Carbon Across Scotland's Coastal Seas
Funding	Scottish Blue Carbon Forum
Staff Responsible	Craig Smeaton
Research Team	<ol style="list-style-type: none"> 1. Craig Smeaton (<i>University of St Andrews</i>) 2. William E.N. Austin (<i>University of St Andrews/Scottish Association of Marine Science</i>)

Metadata Type	Details
Data Resource ID	Geochemical analysis of the quality and reactivity of the organic matter held with the marine sediments of the United Kingdom Exclusive Economic Zone.
Description of dataset	Geochemical data for 885 surficial sediment samples collected from across the Scottish portion of the United Kingdom's Exclusive Economic Zone used to determine of quality and reactivity of the organic matter held with continental shelf sediments.
Locations of the observations	<p>United Kingdom Exclusive Economic Zone</p> <p>Geographic Extent: 61.025808, 3.386188 61.025808, -9.687541 55.265937, 3.386188 55.265937, -9.687541</p> <p>Site locations presented as decimal longitude and latitude (WGS84)</p>
Location Descriptions	The sites were chosen to be represent all major depositional zones on a typical continental shelf these include inshore (fjords and estuaries), coastal (<5 km from land) and offshore (>5 km from land) settings.
Names of the variables or parameters observed or simulated	Folk Classification Labile organic matter (%) Recalcitrant and Refractory organic matter (%) Total organic matter (%) Carbon Reactivity Index (CRI)

	<p>% of total organic matter that is labile % of total organic matter that is recalcitrant and refractory Organic carbon content (%) CN Ratio</p>
<p>All procedures used to make observations or simulations (field/lab where applicable)</p>	<p>Sampling: Archival surficial sediment samples ($n = 434$) were acquired from the British Geological Survey (BGS) sample repository (Keyworth, UK) all obtained from the Scottish portion of the UK EEZ. These samples were described according to the Folk classification scheme (Folk, 1954). Additionally, over a five-year period between 2016-2021, 451 grab and multi-core sediment samples were collected from around Scotland</p> <p>Sample Preparation: Samples were freeze dried and homogenized to a fine powder.</p> <p>Thermogravimetric Analysis: Milled samples of approximately 20 mg were placed into 70 ml aluminium oxide crucibles before being placed into a Mettler Toledo TGA2 and heated from 40°C to 1,000°C at a ramp heating rate of 10°C min⁻¹ under a constant stream of N₂. The thermograms produced from these analyses were adjusted to a common temperature scale and clipped to the range 200-650°C to remove interference from absorbed water and non-organic material. The thermograms were normalized to the mass loss, to assure all thermograms were comparably scaled.</p> <p>Utilizing the TGA data the OM can be grouped into three thermal fractions indicative of lability or biodegradability (Capel et al., 2006). These OM fractions are thermally defined as labile (200 - 400°C), recalcitrant (400 - 550°C) and refractory (550 - 650°C). Using the updated thermal ranges for labile OM (OM_L) (200 - 400°C) and recalcitrant and refractory OM (OM_R) (400 - 650°C) the CRI can be calculated following the Rp Index methodology (Kristensen, 1990). The CRI is calculated as follows:</p> $\text{CRI} = \% \text{OM}_R / \% \text{Total OM}$ <p>Carbon Quantification: Approximately 10 mg of processed sediment was placed into tin capsules and sealed for N analysis. A further 10 mg was placed into a silver capsule; the samples encapsulated in silver underwent acid fumigation to remove carbonate (Harris et al., 2001). The acidified samples were dried for 48 hrs at 40°C and the capsules sealed. The OC and N content of the samples were determined using an Elementar Vario EL following standard methodology (Verardo et al., 1990). The atomic CN ratio was calculated as follows:</p> $\text{C/N} = (\% \text{OC}/12) / (\% \text{N}/14)$
<p>Calibration procedures, where applicable</p>	<p>The elemental analyser was calibrated using Acetanilide. Repeated analysis of medium Organic Soil standard (B2178) during the analysis assured measurement analysis over all analytical runs.</p>

Statistical treatment of the observations or simulations	NA
Data checking procedures (quality control)	All laboratory equipment were calibrated in accordance with the laboratory practises at the University of St Andrews.
File formats used	.csv
Other information	NA indicates no data in cells.

Data resource description for Sedimentary_OC_Quality_Reactivity.csv		
Header	Description	Cell Format
Sample_ID	Sample name	Text
Survey	Survey Identification	Text
Zone	Inshore	Text
	Coastal	
	Offshore	
Latitude	Latitude reported in decimal degrees using the WGS84 projection	Number
Longitude	Longitude reported in decimal degrees using the WGS84 projection	Number
Depth_m	Water depth (m)	Number
Distance_from_land_km	Distance to closest land mass (km)	Number
Sediment_type_folk	Folk Classification (Sediment Type)	Text
OM_L_%	Labile organic matter (%)	Number
OM_R_%	Recalcitrant and refractory organic matter (%)	Number
OM_{total}_%	Total organic matter (%)	Number
CRI	Carbon Reactivity Index	Number
%_of_total_OM_labile	% of total organic matter that is labile	Number
%_of_total_OM_rec_ref	% of total organic matter that is recalcitrant and refractory	Number
OC_%	Organic carbon content (%)	Number
CN	Carbon Nitrogen ratio	Number

References

Capel, E. ., Arranz, J. M., Gonzalez-Vila, F. J., Conzalez-Perez, J. A., & Manning, D. A. C. (2006). Elucidation of different forms of organic carbon in marine sediments from the Atlantic coast of Spain using thermal analysis coupled to isotope ratio and quadrupole mass spectrometry. *Organic Geo*, 37, 1983–1994. <https://doi.org/10.1016/j.orggeochem.2006.07.025>

Folk, R. L. (1954). The distinction between grain size and mineral composition in sedimentary-rock nomenclature. *The Journal of Geology*, 62(4), 344–359.

Harris, D., Horwa, W. R., & Kessel, C. Van. (2001). Acid Fumigation of Soils to Remove Carbonates Prior to Total Organic Carbon or Carbon-13 Isotopic Analysis. *Soil Science Society of America Journal*, 65, 1853–1856. <https://doi.org/10.2136/sssaj2001.1853>

Kristensen, E. (1990). Characterization of biogenic organic matter by stepwise thermogravimetry (STG). *Biogeochemistry*, 9(2), 135–159.

Verardo, D.J., Froelich, P.N. and McIntyre, A., 1990. Determination of organic carbon and nitrogen in marine sediments using the Carlo Erba NA-1500 Analyzer. *Deep Sea Research Part A. Oceanographic Research Papers*, 37(1), pp.157-165.