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Clusters of composition: Elemental content of aquatic organic matter in UK and Faroe peatlands

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ABSTRACT

Water supply companies with reservoirs in peatland areas need to know how land use and vegetation cover in their supply catchments impact the amount and composition of aquatic organic matter in raw waters. Drinking water treatment processes remove organic matter from potable supplies, but recent increases in concentration and changes in composition have made this more difficult. This study analysed the composition of aquatic organic matter from peatland catchments in the UK and Faroe Islands. Both dissolved organic matter (DOM) and particulate organic matter (POM) compositions varied spatially, but these differences were not consistent as water moved through catchments, from headwaters and peatland pools to lake and reservoir outlets. These data showed that lakes and reservoirs are acting as flocculation hotspots, processing OM, releasing carbon (C), hydrogen (H) and oxygen (O) compounds to the atmosphere, and resulting in OM with higher N content. DOM compositions could be grouped into five clusters, showing that water treatment processes can be maximised to target 'envelopes' or clusters of DOM compositions. Catchment factors such as land use, vegetation cover, percentage peat cover and catchment area are good indicators of OM compositions likely to be present in a reservoir, and can guide water companies to maximise efficiency of their raw water treatment processes.

1. Introduction

The composition and concentration of organic matter (OM) in raw water entering drinking water treatment plants from reservoirs is crucially important to the treatment process, especially in the United Kingdom (UK) where approximately 11.4 million people rely on peatlands for their drinking water (Xu et al., 2018). Water companies extract water from highly heterogeneous catchments, across larger geographic areas, and water companies with reservoirs fed by peat catchments have reported the water coming from these sources is harder to treat, often exceeding the capacity of treatment works (Ritson et al., 2014; Tang et al., 2013). In the Faroe Islands, where highly organic soils and peatlands are widespread, drinking water is sourced solely from surface water supplies (Eriksson et al., 2013; Hansen and Aarkrog, 1990; Lawson et al., 2007). Peatlands on the islands have been studied for their accumulation rates (Lawson et al., 2007) and contamination (radiological and perfluoroalkyl substances) (Eriksson et al., 2013; Hansen and Aarkrog, 1990; Shotyk et al., 2005), but very little is known about the impact of these soils on organic matter composition in Faroe raw waters. Water companies in the UK and Faroe Islands need to know how the OM composition in their raw water supplies varies spatially, as it impacts on treatment processes.

Peatlands cover 2.84 % of the Earth, and 13 % of the UK, where fluvial exports are dominated by dissolved organic carbon (DOC) (Billett et al., 2010; Xu et al., 2018). Fluvial DOC fluxes in the northern hemisphere have been increasing since the 1980s, with important implications for carbon budgets (Sawicka et al., 2021) and water treatment (Ritson et al., 2014). DOC is operationally defined as organic carbon in compounds smaller than 0.45 μm. Dissolved organic matter (DOM) is a broader term, and includes other elements present in DOM (e.g. hydrogen (H), nitrogen (N) and oxygen (O)), that are important in DOM processing and availability in water (Kujawinski et al., 2004; Xenopoulos et al., 2021). Particulate organic matter (POM), and DOM are complex mixtures of molecules that vary structurally across a single stream, over time and across catchments and countries (Bowen et al., 2020). The high, and generally increasing, concentrations of OM in water draining from peat and organic soils across the northern hemisphere results in highly coloured water in lakes and reservoirs, which causes problems for water companies that must remove OM from their water supplies (Kothawala et al., 2017). The chemical dosages and energy require to remove DOM from water are expensive, and if the DOM concentration exceeds the treatment plant threshold, treatment plants

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can be shut down, or a new treatment method or plant that costs many tens of millions of dollars is required (Ritson et al., 2016). Water companies are adept at removing the majority of DOM from water, but the process is costly and there are still issues with residual DOM that can react and form potentially carcinogenic disinfection by-products (DBPs). The concentrations of DBPs allowed in drinking water are strictly controlled by water regulations, and water companies must minimise residual DOM during treatment processes (Kothawala et al., 2017).

Water treatment methods are targeted at the normal 'envelope' of OM concentrations and compositions at an individual water treatment works, and include combinations of ozonation, coagulation, sand filtration, anion exchange and granulated active carbon (Kothawala et al., 2017; Lavonen et al., 2015; Sillanpää et al., 2018). Sillanpää et al. (2018) reported that coagulation is not an optimum removal method for natural OM, and Kothawala et al. (2017) showed that anion exchange and granulated active carbon have variable success at removing DOM from water. The success and efficiency of these methods is linked to the composition of DOM (Lavonen et al., 2015; Peacock et al., 2018). DOM composition varies spatially, influenced by land use and vegetation cover, and temporally, influenced by weather and climate, affecting treatment processes (Sillanpää et al., 2018; Tang et al., 2013). Several studies have investigated how both water chemistry factors such as $SUVA_{254}$ (specific absorbance: absorbance at 254 nm per unit organic C); dissolved organic nitrogen, phosphorous and carbon (DON, DOP and DOC) concentrations; trophic status; fluorescence; (e.g. Evans et al. (2017); Hope et al. (1994); Ritson et al. (2016); Sepp et al. (2019); Yates et al. (2022)); and DOM composition factors (such as elemental stoichiometry; e.g. Leifeld et al. (2020); Raeke et al. (2017)) vary in water from peatland areas. Some of these, such as $SUVA_{254}$ and DOC, can be measured directly in the water, whereas others, such as elemental stoichiometry, require OM to be extracted from the water.

Derived elemental composition metrics, including carbon oxidation states, oxidative ratio, and elemental ratios (C/N, O/C, H/C) have shown variation over time and space, and impact on water treatment processes (Lavonen et al., 2015). Physical catchment factors, such as the residence time of lakes and reservoirs, has been shown to affect the variability of DOC reactivity (Catalán et al., 2016; Evans et al., 2017). Water bodies with short residence times had high DOC turnover, due to dominating light-driven removal of OM, whereas longer residence time water bodies were dominated by slower, biological degradation of OM (Evans et al., 2017). Nutrient-rich water bodies had net DOC production, whereas longer residence time water bodies had lower rates of DOC production (Evans et al., 2017). The majority of the above cited studies have focussed on one or two catchment characteristics, or a specific peatland; however, water companies extract water from reservoirs across large areas. Knowledge on how OM varies spatially and with catchment characteristics is therefore important, but currently lacking.

Catchments used for drinking water collection in the UK are managed for multiple purposes, and contain multiple plant functional types and vegetation covers (Billett et al., 2010). Catchments with high percentage peat cover have higher DOC concentrations, and as shown above, residence time, land use and plant functional type impacts OM composition (Sepp et al., 2019). It therefore follows that water draining from small catchments with high percentage peat cover, with land predominantly covered in moorland species (e.g. *Sphagnum* mosses, rough grasses, sedges and heather), that is intensively managed for field-sport of game bird-shooting will have a different OM concentrations and compositions than a large catchment with low peat cover, with improved grasses and used for sheep grazing. Water draining from predominantly forested areas may also have a different OM concentration and composition to that of other areas. There has been a lot of research into how these land management practices alter both the hydrological and carbon cycles of peatlands (Kellerman et al., 2015; Kothawala et al., 2015; Williamson et al., 2021) and much debate about their impact on long-term DOC, OM and water colour trends in surface waters but little research into how catchment characteristics can impact on OM and drinking water treatability across a broad spatial scale.

The primary aim of this study was to understand how composition of OM varies within and across catchments in the UK and Faroe Islands, and if there are common traits that could help water companies characterise and thus treat incoming water, to improve the efficiency of OM removal. The hypothesis that OM from sites in similar areas will have similar compositions will be tested. The second aim was to make recommendations as to how the water industry can make catchment-scale changes to prevent more difficult OM compositions from dominating their raw water sources.

2. Methods

2.1. Study sites

In collaboration with UK water companies, several peatlands and reservoirs were identified for investigation. All fieldwork was carried out during autumn (September to November 2018 and 2019), as the DOC (and therefore DOM) concentrations are typically greatest during this time of year (Clark et al., 2010). In collaboration with the Faroese Geological Survey (Jarðfeingi), water samples were also collected from sites with high organic soil content in the Faroe Islands. The peat soils of the Faroe Islands have been extensively grazed and extracted in the past, and little environmental restoration has taken place (Hagen et al., 2013; Hannon et al., 2001; Lawson et al., 2007). The islands around Scotland have high peat cover and are vulnerable to increasing DOC concentrations (Ferretto et al., 2021), and so these areas were prioritised for water sampling ($n = 185$). In total, 405 individual sites were visited, and water samples were collected and analysed (Fig. 1).

Study sites were located across England ($n = 105$), Scotland ($n = 215$), Wales ($n = 22$), Northern Ireland ($n = 16$) and the Faroe Islands ($n = 47$). Water samples were taken from different water body types located in 177 catchments with peat or organic soils. Water was collected from several locations within each catchment, within access constraints: pools, headwaters, streams and inlets, reservoirs, lakes, and outlets. Peatland pools, with small surface areas and catchment areas, provide useful ecosystems to look at how OM in water varies in these mini-catchments with only one land use and vegetation cover (Chapman et al., 2022). They are also small water bodies, and so can provide much needed data on the aquatic carbon content of these under-studied environments ($n = 30$). Sites that were not reservoirs, lakes or pools were categorised into four groups, according to their location in the catchment: 'headwaters' were typically smaller streams, more than 1 km away from a reservoir/lake; 'inlets' were directly contributing to a sampled reservoir/lake, less than 1 km from the reservoir/lake surface water; 'outlets' were direct output of water, less than 1 km from a sampled reservoir/lake. In some catchments, it wasn't possible to access the reservoir/lake directly; in these catchments water was sampled from 'streams' that did not directly or indirectly contribute to a sampled reservoir/lake. Meta-data for each site and every catchment was assigned at the sample site, derived from site photographs and maps, or found in publically available and published databases for the majority of sites (Supplementary Information, Tables S1 and S2).

2.2. Water sample collection and analysis

At each of the 405 individual study sites, the latitude, longitude and elevation were recorded using a Garmin Oregon 750 GPS. The pH, conductivity, dissolved oxygen and temperature of the water was recorded in situ (Hach MM156 portable multi-parameter meter), along with the air temperature, pressure, and humidity. Photographs were taken at each site to record vegetation cover and land use.

'Grab' water samples were collected at each study site. At every site, a 50 mL water sample was filtered through a 0.45 μm syringe filter (pre-rinsed with deionised water; Sartorius cellulose nitrate membrane filters) in the field. This water was kept as cold and dark as possible: in a

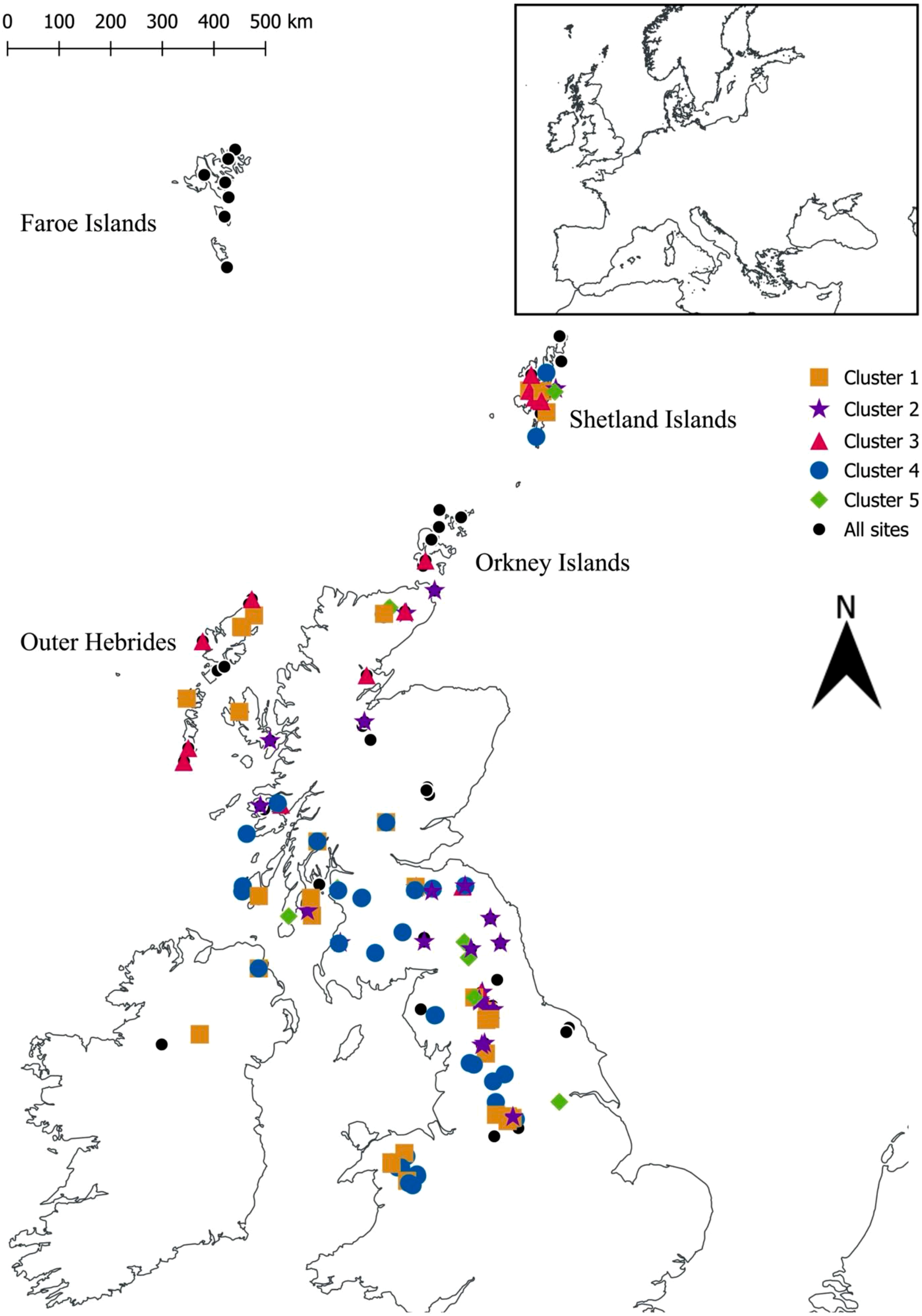

Fig. 1. The location of catchments were water and OM samples were collected. Colours and symbols show the results of cluster analysis on DOM composition. Some sites did not have full OM composition metric data, these sites are shown in black. Insert: the location of the UK and Faroe Islands within Western Europe.

cool bag while in the field, and then a cool box while in transit. The samples were then stored in a fridge at 4 °C in the laboratory and later used to assess water chemistry (within two weeks of sample collection). The dissolved organic and inorganic carbon, absorbance at eight wavelengths and dissolved nutrients, cations, metals and anions were analysed. These measurements were used to derive $SUVA_{254}$, E4/E6,% DON and%DOP ratios for the water samples.

At approximately one third of all sites, a large water sample was collected in a DI-rinsed water caddy ($n = 170$). This water (between 2 and 5 L) was used to study the composition of OM. Water was filtered (VWR glass microfiber filter, 0.7 μm, 47 mm) to extract the particulate organic matter (POM), then the filtered water was rotary evaporated (low pressure, water bath temperature 60 °C max) to concentrate the sample, until approximately 100 mL remained. This small volume of water was placed in an evaporating dish in an oven at 60 °C until all the water had evaporated, and the residue was collected (Moody, 2020). As the water was filtered, the remaining residue was comprised of colloidal and dissolved organic matter (DOM). For further information about water analysis, please see the Supplementary information.

2.3. *OM sample analysis*

Extracted DOM and POM samples were analysed for their elemental composition using an Elementar Vario MICRO cube (total carbon, nitrogen, hydrogen and oxygen, and organic carbon after treatment with hydrochloric acid to remove inorganic carbonates). The proportion of total C that was organic C was calculated (%C_{org}). The total carbon, nitrogen (N) and hydrogen (H) content of the OM samples were used to calculate the C/N ratio, and the double-bond equivalent (DBE, also known as degree of unsaturation) of each sample (Equation 1, SI). The DBE was 'normalised' to the total number of C atoms in a molecule (DBE/C) to avoid larger molecule size affecting the result. For molecules comprised solely of C and H, the DBE/C varies from 0 to 1. However, the OM samples in this study are not solely C and H and therefore the DBE/C can fall outside this range. Koch and Dittmar (2006) explained how introducing N and O atoms into molecules changes the potential bonding but would not necessarily change the DBE/C value, and so DBE/C can only be a guide to structure. DBE has been shown to be negatively related to the rates of microbial respiration in water (Hu et al., 2023), and compounds with high DBE were preferentially photo-degraded when water samples were exposed to light (Kujawinski et al., 2004). In a study of drinking water treatment processes, Phungsai et al. (2018) used a slightly different measure ((DBE-O)/C) to show samples with less unsaturated DOM had the largest changes when undergoing ozonation, and more saturated compounds increased. Their water samples had higher (DBE-O)/C after drinking water treatment (Phungsai et al., 2018).

The C, H, N and O content of OM samples were used to calculate H/C and O/C ratios, and the carbon oxidation state (C_{ox}) and oxidative ratio (OR) (Equations 2 and 3 in SI, from Hockaday et al. (2009). An increase in the C_{ox} reflects an oxidation reaction, while a decrease is a reduction reaction. The OR is the ratio of moles of O_2 released to CO_2 sequestered in the terrestrial biosphere – in terms of OM, this means O_2 release when CO_2 is sequestered into organic matter when formed, either from plants, soil or produced by microbes. The C_{ox} and OR metrics are usually inverse – samples with high OR have low C_{ox} and vice versa. Carbon oxidation state was considered in a study of natural organic matter and drinking water treatment, where carbon oxidation was shown to be useful for separating terrestrial and in-lake produced DOM, and compounds with high C_{ox} decreased in abundance after coagulation treatment (Lavonen et al., 2015). For more details of OM analysis, see Supplementary Information.

2.4. *Statistical analysis*

All statistical analysis was carried out using SAS 9.4. The DOM and POM composition metrics were tested for normality, transformed if necessary, and analysed. As there were several different ways of classifying the data, (e.g. type of water body, land use, vegetation cover, level of disturbance), and several OM metrics, Principal Component Analysis (PCA) and Cluster Analysis were used to determine which factors were important in determining OM metrics. PCA used seven derived metrics (C_{ox}, OR,%C_{org}, DBE/C, C/N, H/C, O/C) for OM. Graphs of PC1 vs PC2 were plotted, with samples grouped using each category (e.g. by land use, or by vegetation cover). The PC loadings were analysed using several one-way ANOVA, with the categorical values as factors. *Post-hoc* Duncan's multiple range tests were used if ANOVA showed significant differences. Simple linear regressions were used to look at relationships between PC loadings and continuous variables (e.g. latitude, longitude, elevation, water chemistry variables), and were reported as significant if $p < 0.05$. For regression analysis, adjusted R^2 values are reported. For cluster analysis, variables were z-scored, then grouped into clusters based on OM composition metric similarities. Ward's method of hierarchical cluster analysis uses minimum variance between samples to determine clusters. The pseudo F and cubic clustering criterion were used to determine the number of clusters: for DOM metrics this was determined to be five clusters, for POM this was three clusters.

Results sections 3.1 to 3.6 consider all samples, regardless of region of origin; however the Faroe Island OM samples did not have a full complement of DOM or POM derived metric data. Therefore they were not included in PCA or cluster analysis approaches. They are discussed in section 3.7 (and in SI), where the composition of OM samples collected in the Faroe Islands were compared to those collected in the UK.

3. Results

The majority of water samples were 'typical' of peatland waters (Table 1); they were acidic (mean pH 5.47) and had low electrical conductivity (mean EC 218 µS cm^{-1}). They were organic carbon rich (high DOC and POC; mean DOC 16.2 and mean POC 1.7 mg C l^{-1}), and nutrient poor (low DON and DOP; mean DON 0.55 mg N l^{-1} and mean DOP 13.3 µg P l^{-1}).

The four measured elements (C, H, N and O) accounted for up to 91 % of the DOM and 96 % of the POM mass. The majority of the mass was carbon (up to 43 % of DOM and 45 % of POM samples). C/N ratios of DOM varied from 2 to 101, and from 3 to 41 for POM, indicating a wide variety in the number of C moles per N mole, especially for DOM samples (Table 2). OM H/C values ranged from 0.6 to 3.9, O/C values ranged from 0.1 to 1.9. The mean double bond equivalence (DBE/C) was 0.97 for DOM and 1.04 for POM – on average the DOM samples had fewer double bonds per carbon than POM. Carbon oxidation state (C_{ox}) values ranged from −1.6 to 3.9, and oxidative ratios (OR) ranged from 0 to 1.4. The lowest%C_{org} was 16 % in DOM, and 28 % in POM.

There were ten catchments with DOM and POM samples taken from the inlet, reservoir/lake water and outlet of a reservoir/lake. In these catchments, the mean C/N ratio of DOM fell from 41 in the inlets to 35 in the outlets, and the DBE/C ratio increased from 0.87 to 1.02. Based on elemental stoichiometry of DOM, there was a loss of $C_{11}H_{12}O_5$ between the inlet and outlet of the lake/reservoirs (normalised to 1 mole of N). In these 10 catchments, the mean C/N ratio of POM fell from 16 in inlets to 12 in outlets, and the DBE/C ratio increased from 1.10 to 1.37. Based on elemental stoichiometry of POM, there was a loss of $C_5H_6O_4$ between reservoir/lake water and outlet of the lake/reservoirs (normalised to 1 mole of N).

Table 1
Mean, minimum, maximum, median and n of water chemistry variables. EC=electrical conductivity; DO=dissolved oxygen; $SUVA_{254}$= absorbance at 254 nm divided by DOC concentration; E4/E6=absorbance at 465 nm divided by 665 nm; DOC=dissolved organic carbon; DON=dissolved organic nitrogen; DOP=dissolved organic phosphorous; POC=particulate organic carbon;% DON=proportion of total N that is organic;%DOP=proportion of total P that is organic.

Variable	n	Minimum	Maximum	Mean	Median
pH	402	3.83	10.02	5.47	6.72
EC µS cm^{-1}	432	16.07	2990.00	218.28	99.25
DO%	327	20.00	189.10	92.07	93.00
$SUVA_{254}$ L mg^{-1} m^{-1}	397	0.24	9.63	4.10	4.25
E4/E6	393	0.77	14.38	6.00	5.97
DOC mg C l^{-1}	405	0.06	95.20	16.15	13.45
DON mg N l^{-1}	179	0.00	1.87	0.55	0.49
DOP µg P l^{-1}	183	0.00	87.50	13.29	9.00
POC mg C l^{-1}	145	0.10	14.61	1.70	0.83
%DON	179	2.00	97.91	75.27	80.61
%DOP	182	0.00	100.00	62.59	68.21

Table 2
Mean, minimum, maximum, median and n of derived OM composition metrics. DOM=dissolved organic matter; POM=particulate organic matter;%C_{org}=proportion of total C that is organic; C/N=carbon/nitrogen ratio; C_{ox}=carbon oxidation state; DBE/C=double bond equivalent per carbon; H/C=hydrogen/carbon ratio; O/C=oxygen/carbon ratio; OR=oxidative ratio.

OM	Variable	N	Minimum	Maximum	Mean	Median
DOM	%C_{org}	170	0.16	1.09	0.81	0.86
	C/N	171	1.85	101.11	34.59	34.59
	C_{ox}	153	0.13	3.97	1.24	1.06
	DBE/C	160	0.57	2.33	0.97	0.88
	H/C	151	0.56	3.99	1.74	1.66
	O/C	136	0.74	1.97	1.22	1.18
	OR	153	0.06	0.98	0.72	0.76
POM	%C_{org}	65	0.28	1.09	0.94	0.97
	C/N	165	2.62	41.28	15.47	14.26
	C_{ox}	64	−1.58	3.95	0.50	0.37
	DBE/C	146	0.07	2.89	1.04	0.90
	H/C	142	0.64	3.46	1.99	1.92
	O/C	62	0.10	1.87	1.10	1.12
	OR	64	0.08	1.44	0.92	0.96

3.1. DOM PCA

The principal component analysis (PCA) on DOM composition used 124 samples with full C_{ox}, OR,%C_{org}, DBE/C, C/N, H/C, O/C metrics. The first three components explained 85.2 % of the variation (Table 3). PC1 (47.1 % of variation) was strongly driven by oxidation gradient, with high positive values for DOM with high C_{ox} and O/C, and negative OR (Fig. 2). PC2 (21.1 %) had high positive values for DOM samples with high H/C.%C_{org} and C/N ratio of DOM had high positive and negative loadings, respectively, for PC3 (17.0 %).

The PC loadings for all DOM samples were analysed by one-way ANOVA, using area, type, land use, vegetation cover, level of disturbance and position as factors. Factors that are strongly linked to geographic position (such as area and position; Fig. S1A) showed significant differences in all or almost all of the components, explaining between 6 and 45 % of the variation (Table 3). There were significant differences in PC loadings for components 1, 3, 4 and 5 between water body types (Fig. S1B). Land use was only significant in PC3 (driven by C/N content of DOM; Fig. S1C), and vegetation cover was only significant in PC1–3 (Fig. S1D). There were no significant differences in PC loading between sites with different levels of disturbance.

This analysis shows there are multiple differences between DOM composition metrics in samples collected from across the UK and Faroe Islands. Sites with highly organic DOM, with high OR values (low PC1) were generally from the southern end of the sampling area, moorland areas, with bog or heather cover, used for grazing or shooting, with small catchment areas. Sites with highly saturated and oxidised DOM (high PC1) were from more northern areas, often on woodland or grasses, used for plantation, grazing or renewable energy (wind turbines or hydropower). Sites with highly organic, unsaturated DOM (low PC2) were on mainland, woodland or bog areas, with mixed land use and water body type. Sites with highly saturated DOM (high PC2) were from islands, northern streams, with HG ('heather grass') cover, used for peat cutting or renewables. Sites with high C/N DOM (low PC3) were generally lake or reservoir inlets, with plantation land use. Sites with highly organic DOM (high PC3) were wooded reservoir surface waters or outlets.

3.2. DOM cluster analysis

There were five clusters of DOM samples, based on similarities in DOM composition metrics (Figs. 1 and 3). In total, 123 DOM samples were included in this analysis, 35 from islands, and 88 from mainland sites. There are several occasions when all, or nearly all, samples from within the same catchment, or same island, are grouped in the same cluster, even though they have different land uses, vegetation covers, catchment areas and they are from different water bodies within that catchment. In cluster 1 ($n = 33$), there were 11 DOM samples from four different island groups, whereas cluster 2 ($n = 27$) only contained three island DOM samples. The majority of samples in cluster 3 were from islands at high latitudes, while cluster 4 was mainly mainland, lower latitude DOM samples. Cluster 5 was the smallest cluster ($n = 11$), and only one of those was from an island.

3.3. DOM cluster and PCA

The average PC loadings for each cluster are shown in Fig. 4. They show clear differences in PC loadings based on cluster groupings. An ANOVA on the PC loadings, with cluster as a factor, showed good agreement between the two methods – there were significant differences in all PC components between clusters, with R^2 values of 0.79, 0.48 and 0.41 (explaining up to 79 % of the variation). Clusters 3, 4 and 5 have relatively similar PC1 loadings, and are significantly lower than cluster 2, and higher than cluster 1. Clusters 3 and 5 are the highest and lowest PC2 loadings, significantly different to clusters 1, 4 and 2. These two methods show that despite the range of latitude, longitude, elevation and catchment characteristics included in this study, DOM composition can be broadly grouped into five different groups, based on metrics derived from relatively simple elemental analysis.

3.4. POM PCA

Similar to the PCA on DOM, the PCA on POM samples ($n = 43$ with all composition metrics) showed the majority of variation was explained by the first three components (89 %, Table 4). The PC loadings were also similar to the results for DOM samples, where PC1 (48.6 % of variation) was driven by an oxidation gradient, with high positive values for POM samples with high O/C and C_{ox} values, and low OR values (Fig. 5). PC2 (26.4 %) was determined by saturation, with high H/C and low C/N values. PC3 (14 %) was also driven by the%C_{org}.

The PC loadings for all POM samples were analysed by one-way ANOVA, using area, type, land use, vegetation cover, level of

Table 3
The eigenvalue and proportion of variation explained by Principal Component Analysis (PCA) on DOM metrics, and ANOVA on Principal Components 1–6 (PC1-PC6) ($n = 124$). Variation explained (r^2) values reported for significant ($p < 0.05$) values. ANOVA results were not significant ($p > 0.05$) for all components when looking at disturbance.

	PCA		ANOVA on…									
	Eigenvalue	Prop.	Area		Water body		Land use		Veg. cover		Position	
			p	r^2	p	r^2	p	r^2	p	r^2	p	r^2
PC1	3.30	0.47	0.0013	0.30	0.0247	0.14	0.2729		0.0086	0.13	0.6118	
PC2	1.48	0.21	0.0010	0.30	0.3618		0.1347		0.0468	0.10	0.0001	0.15
PC3	1.19	0.17	0.0002	0.33	0.0010	0.20	0.0275	0.14	0.0291	0.11	0.0083	0.06
PC4	0.66	0.09	0.0029	0.28	0.0407	0.13	0.1671		0.0948		0.0064	0.06
PC5	0.38	0.05	0.0001	0.45	0.0291	0.13	0.0941		0.7233		0.0001	0.16
PC6	0.00	0.00	0.0009	0.30	0.7441		0.4525		0.8798		0.9503	

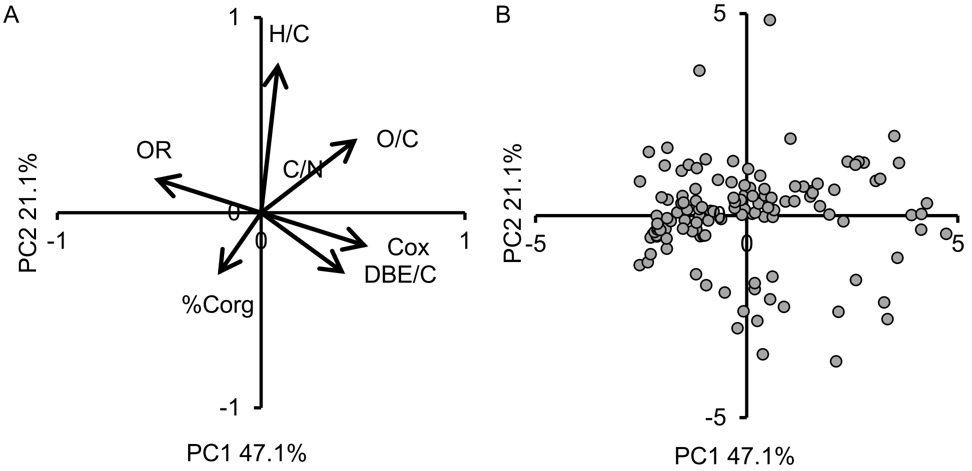

Fig. 2. A) The loadings for each metric included in the PCA on DOM composition. Loadings for C/N were (−0.004, 0.004) too close to the origin to show an arrow. B) The loadings for each DOM sample for components 1 and 2.

disturbance and position as factors (Table 4). These results differed from those for DOM samples; for POM, there were relatively few significant differences, showing that the majority of variation in POM composition was not associated with these factors.

As none of the factors analysed could fully explain the variation in POM composition metrics, PC1, PC2 and PC3 loadings were modelled using continuous variables (e.g. latitude, water chemistry variables,% peat cover) in linear regressions (Table S2). There was one significant relationship for PC1 loadings (Fig. S2A): a significant positive relationship with $SUVA_{254}$ (adj. $R^2 = 0.11$). As $SUVA_{254}$ is considered a proxy for aromaticity of OM (Hu et al., 2023), it is possible that PC1 reflects the aromaticity of the compounds in POM, rather than catchment characteristics. There were three significant linear relationships between PC2 loadings: DOC (adj. $R^2 = 0.21$),% peat cover (adj. $R^2 = 0.16$), and $SUVA_{254}$ (adj. $R^2 = 0.09$). Sites with a high percentage peat cover and high DOC concentrations had low PC2 loadings, indicating the POM from these sites had high C/N and low H/C ratios. The relationship between $SUVA_{254}$ and PC2 was the negative: samples from sites with high $SUVA_{254}$ values had high PC1 loading and low PC2 loadings, indicating high O/C and C_{ox}, and high C/N. As shown in the ANOVA on area (Table 4), there was a significant relationship between PC3 loadings and longitude (adj. $R^2 = 0.08$); POM samples from sites to the west had low PC3, indicating high DBE/C, and sites from the east had high% C_{org} values. Further details about these relationships can be found in the Supplementary Information.

3.5. POM cluster analysis

There were three clusters of POM samples, based on similarities in POM composition metrics (Fig. 6). As there were fewer POM samples with all seven composition metrics needed for this analysis, there were only 40 POM samples included.

3.6. POM cluster and PCA

The PC loadings for each cluster are shown in Fig. 7. Similar to the results for DOM samples, they show clear differences in PC loadings based on cluster groupings. An ANOVA on the PC loadings, with cluster as a factor, showed good agreement between the two methods – there were significant differences in PC1 and PC2 components between clusters, with R^2 values of 0.70 and 0.56 (explaining up to 70 % of the variation). Clusters 2 and 3 have relatively similar PC1 loadings, and are significantly higher than cluster 1. Cluster 3 had the lowest PC2 loadings, significantly lower than clusters 1 and 2. Combining these two methods shows that cluster analysis explains up to 70 % of the variation in PC1 loadings, whereas none of the factors analysed in section 3.4 and Table 4 had significant relationships with PC1.

3.7. Comparison of Faroe Island and UK samples

The POM in Faroe waters was less oxygenated and had fewer double bonds per carbon (lower C_{ox}, DBE/C and O/C), and was more saturated with hydrogen (higher OR, H/C) than in UK samples. The C/N and% C_{org} in Faroe POM were similar to UK samples. Faroe DOM was more oxygenated (higher C_{ox}, lower OR) and less saturated (higher DBE/C) than UK DOM. The Faroe DOM also had lower C/N ratios than UK DOM, indicating more N-rich compounds than in UK samples.

Both the water chemistry and OM composition results show the samples from the Faroe Islands were derived from soils with lower organic content than UK peatlands, with a significant marine influence. As little restoration work has been undertaken in the Faroe Islands, these results and analogies with UK sites could be used to show which areas of the Faroe Islands might benefit from changes in environmental management, leading to ecological improvements (Hagen et al., 2013; Hannon et al., 2001; Lawson et al., 2007).

4. Discussion and implications for water treatment

4.1. How does the OM composition change spatially?

Both DOM and POM compositions varied spatially both between and within catchments, but these changes were not consistent across latitude or longitude, or from headwater and peatland pool to lake and reservoir outlets. DOM samples from similar locations (e.g. within the same catchment, or on the same island) often grouped together in the cluster analysis, demonstrating that clustering DOM samples by composition metrics has benefits over categorising by e.g. land use or water body type, and supporting the hypothesis that OM from sites in similar areas will have similar compositions. These clusters represent compositionally similar DOM that would react similarly during water treatment processing. This could benefit water companies, to be able to maximise treatment efficiency for an envelope of DOM compositions. Water companies with catchments that are at high elevations, small catchment areas and located further west would have DOM with lower O content (cluster 1), whereas water in catchments located further east, in larger catchment areas, with low peat cover, had DOM with high O content (cluster 2). As O-rich compounds can be easily removed by coagulation during drinking water treatment (Wilske et al., 2021), these results show coagulation would effectively remove DOM in cluster 2 samples, but would be less effective on cluster 1 samples.

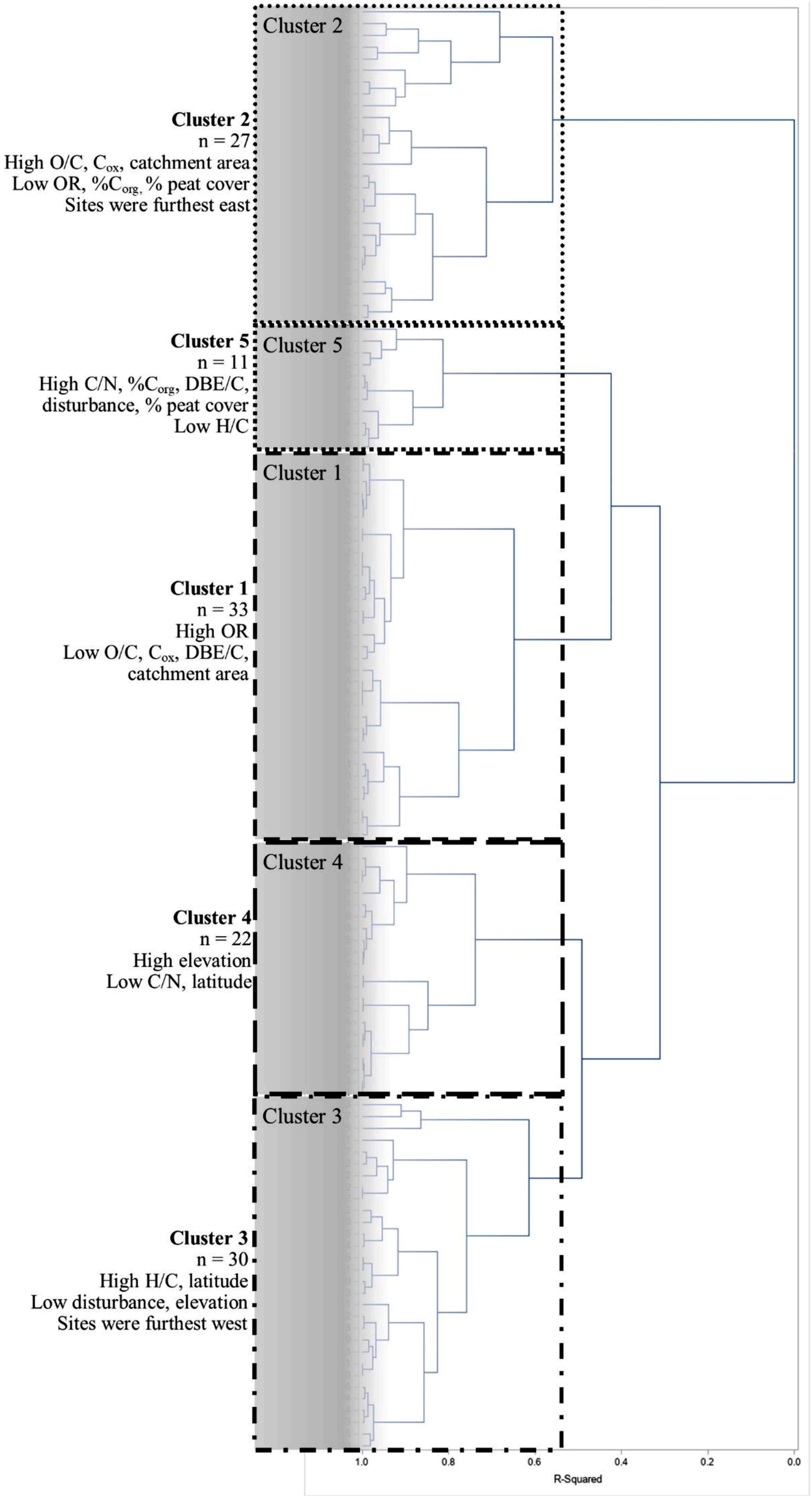

Fig. 3. The results of cluster analysis on DOM composition metrics, with clusters and their common traits shown. Tree line length shows similar samples. Identities of samples are greyed out to keep source waters anonymous to comply with water company requirements.

Composition varied within catchments: both DOM and POM became more oxidised as the water travelled through catchments. Composition metrics showed that the proportion of organic carbon, the number of double bonds per carbon in a molecule, and the hydrogen, oxygen and nitrogen content of both DOM and POM varied spatially within catchments. These changes would result in OM with different elemental composition and structures along the water continuum, reflecting in-stream processing of OM. There were differences between natural (e.g. lakes and lochs) and artificial (reservoir) water bodies – DOM and POM from lakes had higher C/N and lower$\%C_{org}$ than DOM and POM from

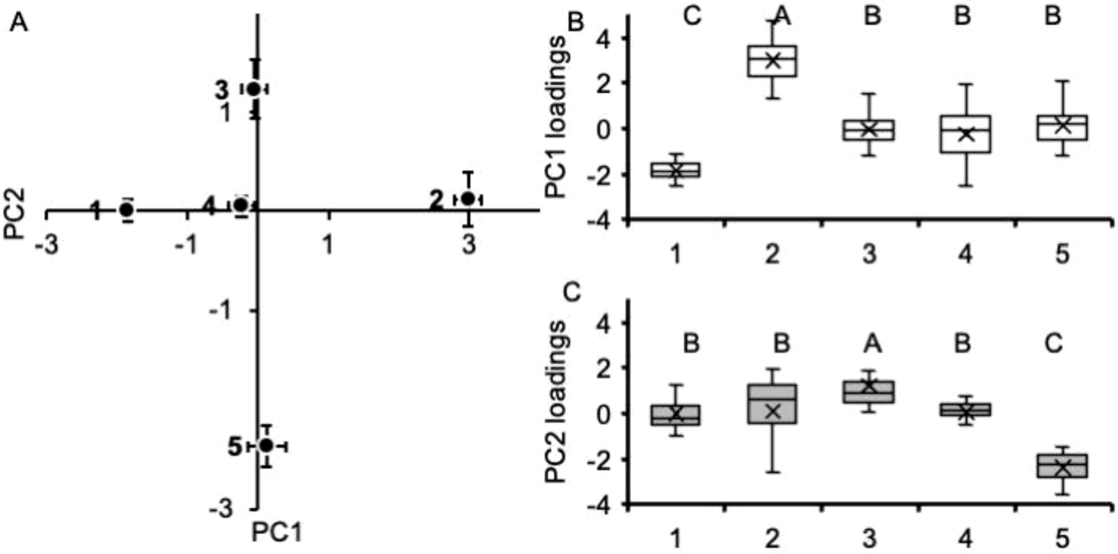

Fig. 4. A) The mean average (black circle) and standard error of PC1 and PC2 loadings for each cluster of DOM compositions. Box plots for B) PC1 and C) PC2 loadings for clusters 1–5, where horizontal lines are median values and the 'X' show the mean values. Letters indicate significant differences between clusters in a one-way ANOVA.

Table 4
The eigenvalue and proportion of variation explained by Principal Component Analysis (PCA) on POM metrics, and ANOVA on Principal Components 1–6 (PC1-PC6) ($n = 43$). Variation explained (r^2) values reported for significant ($p < 0.05$) values. There were no significant results for ANOVA on land use or veg cover ($p > 0.05$ for all PC components). The r^2 values for the few significant relationships are larger than those for DOM due to the lower number of POM samples with a full set of composition metrics for this analysis.

	PCA		ANOVA on…							
	Eigenvalue	Prop.	Area		Water body		Position		Disturbance	
			p	r^2	p	r^2	p	r^2	p	r^2
PC1	3.40	0.49	0.3257		0.3808		0.8333		0.3334	
PC2	1.85	0.26	0.8357		0.0193	0.36	0.9022		0.4486	
PC3	0.98	0.14	0.0011	0.74	0.8214		0.9232		0.0785	
PC4	0.49	0.07	0.0271	0.64	0.8742		0.0153	0.14	0.0297	0.24
PC5	0.28	0.04	0.1937		0.2260		0.1435		0.3160	
PC6	0.00	0.00	0.0279	0.63	0.9651		0.4475		0.4416	

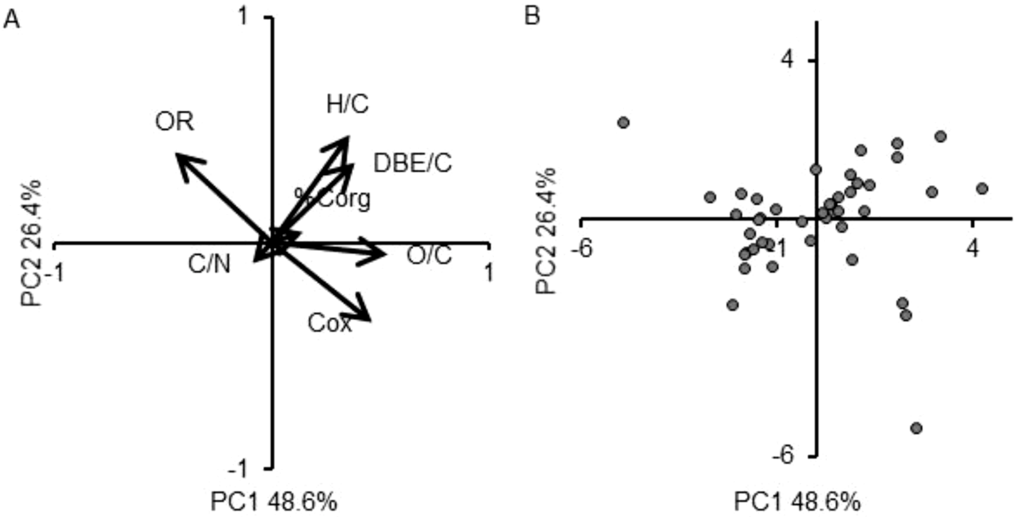

Fig. 5. A) The loadings for each metric included in the PCA on POM composition. B) The loadings for each POM sample for components 1 and 2.

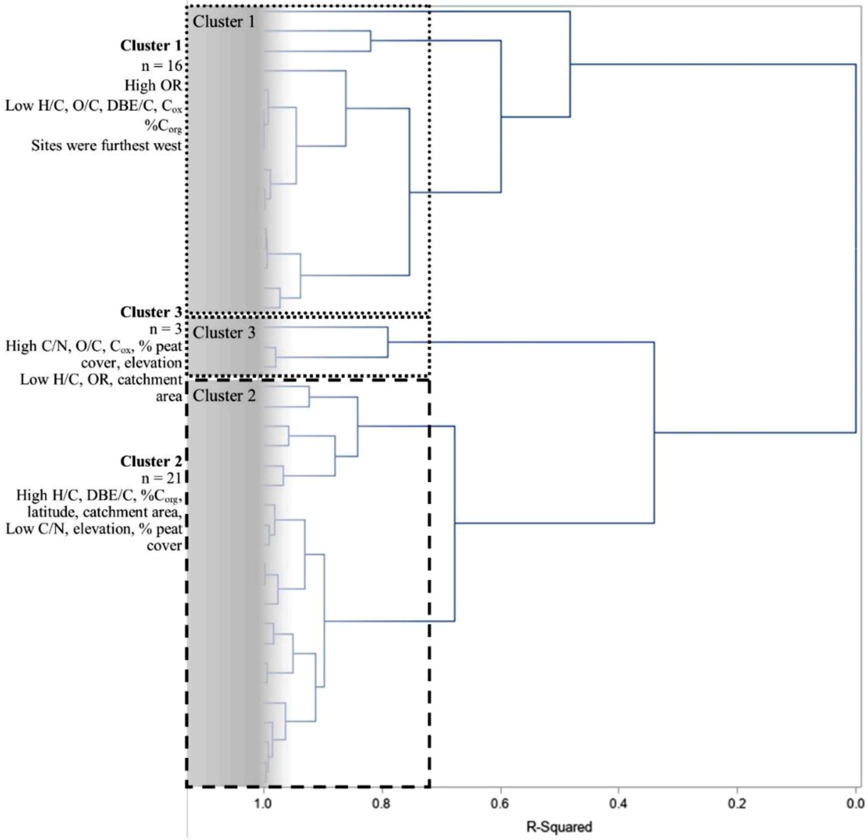

Fig. 6. Results of cluster analysis of POM samples, showing clusters and main traits of each cluster, based on seven derived POM composition metrics. Tree line length shows similar samples. Identities of samples are greyed out to keep source waters anonymous.

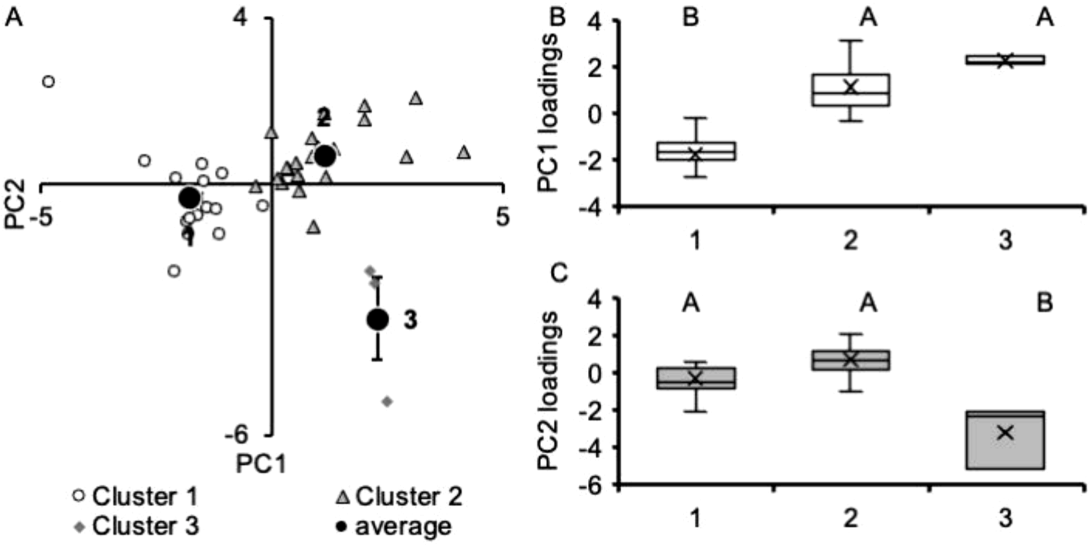

Fig. 7. A) The PC1 and PC2 loadings for each POM sample, grouped by cluster, and the mean average (black circle) and standard error of PC1 and PC2 loadings for each cluster of POM compositions. Box plots for B) PC1 and C) PC2 loadings for clusters 1–3, where horizontal lines are median values and the 'X' show the mean values. Letters indicate significant differences between clusters in a one-way ANOVA.

reservoirs. Impounding a water body changes the hydrology, increasing water residence time, and there are several catchment characteristic differences between lakes and reservoirs (Hayes et al., 2017). Lakes/reservoirs that are deep or have large surface areas (and therefore contain a high volume of water), are likely to have longer residence times than smaller, shallow lakes. The mean catchment area of reservoirs was 32 km^2 whereas lake catchment area was significantly smaller at 9.6 km^2 in this study, which would account for some of the differences between lakes and reservoirs. Hayes et al. (2017) also determined that, globally, latitude was important in the differences between lakes and reservoirs – reservoirs can occur at any latitude whereas lakes tend to occur at high latitudes. This was also true of sites in this study; the mean latitude of lakes was significantly higher, at 57.9° N, whereas for reservoirs it was 54.9° N (one-way ANOVA, $p < 0.01$, $R^2 = 0.17$). Both lakes and reservoirs actively process OM inputs, and are hotspots of microbial degradation, autochthonous primary production, photodegradation and sedimentation (Tranvik et al., 2009). This study found that although there were differences between lakes and reservoirs (e.g. C/N content of DOM and POM), the differences in OM composition between lakes/reservoirs and their headwaters was greater. The reservoirs/lakes are 'buffering' changes in OM, storing C, H and O in POM and DOM, but releasing OM with higher N content. This suggests that in-lake production of DOM (e.g. by microbes and algae), and in-lake production of POM (e.g. by flocculation of DOM, production by algae), results in OM with higher N content and decreased C_{ox} values (Lavonen et al., 2015). The DOC and POC concentrations were also different at different locations, suggesting variable OM inputs and processes. Flocculation of DOM to POM would account for higher POC concentrations in lakes and reservoirs than inlets and headwaters (Chapman et al., 2022; Von Wachenfeldt and Tranvik, 2008), and in-situ production of OM (by microbes and algae) resulted in OM with high N content. These show that lakes and reservoirs are acting as flocculation hotspots, processing OM, releasing C, H and O compounds to the atmosphere, and releasing OM with higher N content.

DOM from larger catchments (clusters 2 and 4) was more oxidised, less saturated and had lower C/N ratios than water from smaller catchments (cluster 1). Studies have shown the C/N ratio of water is important for treatment – higher N content (OM with low C/N) increases chlorine demand during chlorination and increases formation of DBPs (tri-halomethane compounds) that are difficult to remove (Peacock et al., 2018; Ritson et al., 2014, 2016). This study showed headwaters in small, northern catchments, where the sites had bog, heather or 'heather grass' cover, where the land was used for generic moorland, or restored peat, had the highest C/N ratios of DOM (high carbon, low nitrogen). Land uses with low C/N included moorland used for game shooting or sheep grazing, and felled forest. These land uses disturb the peat, and risk exposing larger surface areas of peat to drying out, increasing degradation by light and microbes, reduces the carbon store of peatlands, and can cause irreversible damage to peat-forming vegetation. The remaining peat left behind after disturbance is more susceptible to further degradation and erosion (Blundell and Holden, 2019; Swindles et al., 2016). To lower the N content of DOM (increase the C/N ratio), the best strategy would be to reduce disturbance by restoring peatland – DOM from restored sites had higher C/N than from grazed and felled sites, and restoration brings multiple benefits (e.g. increase C and water storage, increased biodiversity) to peatland sites (Billett et al., 2010).

The oxidation status of OM in water has implications for drinking water treatment processes. Lavonen et al. (2015) found coagulation treatment selectively removed terrestrial DOM – that is highly oxidised (high C_{ox} and O/C), aromatic (high $SUVA_{254}$), and unsaturated (low H/C). Sand filtration selectively targeted DOM from autochthonous (in-situ) sources, with more reduced (low C_{ox}), highly saturated (high H/C), relatively few double bonds (low DBE/C) and low oxygen content (low O/C). The present study has shown that large catchments at high latitudes had DOM with high C_{ox}, O/C and DBE/C. The results of Lavonen et al. (2015) suggest this DOM would readily be removed during coagulation treatment, whereas DOM from bog and heather sites had low C_{ox}, O/C and DBE/C, and would need sand filtration to be removed from drinking water supplies. Phungsai et al. (2018) used a measure of DBE including oxygen content ((DBE-O)/C) showing that samples with less unsaturated DOM underwent large changes when exposed to ozone water treatment. Calculating this variable for the DOM samples in the present study showed it had a negative relationship with DBE/C ($p < 0.01$, $R^2 = 0.23$), indicating that samples with high DBE/C would have lower DBE/C after treatment with ozone. These results show that treatment processes can be maximised to target different OM compositions. Factors such as land use, vegetation cover, percentage peat cover and catchment area can give indicators of the OM compositions likely to be present in a reservoir, allowing water companies to maximise efficiency of their raw water treatment processes accordingly. If water companies want to manipulate OM compositions in their reservoirs, modifying environmental management (land use and vegetation cover) could yield changes in OM composition, as shown by relationships between plant functional type and OM composition.

4.2. *Implications for water treatment*

Water companies need to know the 'treatability' of their incoming raw water in each water treatment works in order to set them up to effectively remove the OM. The results of this study have shown some general patterns that could help water companies determine how best to treat their incoming water, depending on the location and characteristics of their raw water supplies. These results show that sites with large catchment areas and low peat cover, will have highly oxidised DOM and highly saturated POM (cluster 2 in both DOM and POM cluster analysis). Sites with high peat cover will have highly organic DOM (DOM cluster 5) and highly oxidised POM (POM cluster 3). Sites at high elevation will have DOM with low oxygen content (DOM cluster 1) and POM with high C/N (POM cluster 3). Sites at high latitudes have DOM with high C/N (DOM cluster 3) and highly saturated POM (POM cluster 2). Knowing the OM traits likely to occur in raw water supplies will allow water companies to target treatment processes to remove more efficient removal of OM.

For water companies, these results show that extracting water from lakes and reservoirs means they will be taking in raw water containing OM with high N content (low C/N), which is subsequently more difficult to remove during treatment processes (Raeke et al., 2017). A possible conclusion from this study could be that water companies change water sources within a catchment, moving from extracting water from a reservoir to a stream or headwater, to change the incoming composition of DOM. However, the inconsistent flow rates of headwaters and streams, alongside the considerable infrastructure requirements and increasing water demands make this very challenging in many instances. There are also risks associated with extracting water from running water (e.g. *Cryptosporidium* (Betancourt and Rose, 2004). In reservoirs where intakes from incoming streams and rivers can be temporarily 'switched off' (e.g. water flow diverted away from reservoirs), the findings presented herein could inform source appointment decisions. As shown, catchment characteristics can affect OM composition in these stream and river inputs, and so modifying which inputs contribute to a reservoir could change the composition of OM within the reservoir, although these changes could take a long time to impact reservoir OM given the longer residence times of reservoirs. Modifying environmental management within catchments (such as peatland restoration) or nutrient inputs could also be used to manipulate OM composition within a reservoir, and could be more cost effective than building new treatment plants (Ritson et al., 2016).

The differences in OM composition between water body types (especially lakes and reservoirs), vegetation cover and land-use categories, alongside physical location, could help water managers plan locations for building new reservoirs. For example, there were significant relationships between latitude and oxidative state (C_{ox}, OR, O/C) and structural (C/N, DBE/C) metrics of DOM, and between percentage peat and all DOM composition metrics; these results could help determine OM inputs at potential new reservoir locations.

5. Conclusion

Organic matter was extracted from water samples collected from peatland and organic soils sites across the UK and Faroe Islands. Results showed significant variation spatially, and between lakes and reservoirs, between land uses and vegetation covers. This paper provides evidence for using catchment-based environmental management solutions, such as peatland restoration, to modify OM compositions, which could be used to mitigate against longer-term change and reduce the need for more costly capital interventions in new treatment facilities. The findings suggest that water companies can use catchment characteristics as indicators of OM composition likely to be present in a reservoir, and therefore target specific types of OM and maximise treatment efficiency. Water company investment in catchment design could be tailored to alter catchment characteristics, such as changing land use and/or vegetation cover, to modify OM into compositions that are easier to treat (e.g. restoring peatland areas by reducing disturbance to raise C/N ratios of DOM in raw water). Treatment operations could also be tailored to incoming OM compositions, to maximise treatment efficiency, for example by using coagulation rather than sand filtration where OM is highly oxidised.

CRediT authorship contribution statement

Catherine S. Moody: Writing – review & editing, Writing – original draft, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

DOI for the data is in the manuscript

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The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary materials

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