Reconstruction of Holocene sea-levels using diatom- and pollen-based microfossil transfer functions, west coast of Scotland, UK

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This thesis is dedicated to my late grandfather Frederick Evans without whose contagious love of nature and the natural world I would not have been driven to learn about the environment. I wish he could be here to see me complete my thesis

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ABSTRACT

Due to its sensitivity to isostatic and eustatic sea-level change the west coast of Scotland has been an important area for studying sea-level change. Recently, data from north west Scotland have been used to refine GIA models because of the presence of the ice sheets of the last glacial maximum (LGM) and its long record of sea-level change exceeding 10 000 yr. The Holocene highstand record of the area studied in Scotland is preserved within the many isolation basins, tidal marsh sediments and raised beaches which collectively preserve a diachronous record of marginal marine sedimentation over the course of the Holocene. The Arisaig area preserves one of the longest records of relative sea-level change in Great Britain, in excess of 16 ka (e.g. Shennan *et al.*, 1993, 1994, 1995a and 1995b). The microfossil sediment sequence from Mointeach Mhor North, is an important bio-stratigraphical sequence from the north west coast because it records both the rise and fall of sea level throughout the mid Holocene more precisely than many other sites.

Where until recently the data used to reconstruct RSL were sea level index points taken from regressive and/or transgressive contacts, verified by the microfossil data, this investigation aims to for the first time reconstruct sea-level change through the sediment sequence using diatom, pollen and multi-proxy microfossil-based transfer functions.

This thesis also highlights some of the problems encountered associated with the transfer function technique and microfossil choice that may limit or constrain the applicability of transfer functions in sea-level studies, including spatial autocorrelation, over- and under-estimation of optima, multiple analogues, no analogues and the problem of allochthonous and autochthonous species.

This research project has determined that regional and local multi-proxy transfer functions have the potential to reconstruct reference water levels (RWLs) more precisely than diatom and pollen training sets (Table 4.16). When the regional transfer functions were ran again using only the samples

within the multi-proxy training set to allow direct comparison, the multi-proxy training set still produced the best performance statistics. When the training sets were used to calibrate the fossil cores/monoliths to produce estimates of RWL (Chapter 6) the original samples containing all available samples gave more sensible and reliable estimates of RWL than the training sets that only contained the 75 assemblages in the multi-proxy training set. In Chapter 6 the original regional diatom training set produced the most reliable and sensible estimates of RWL. The excellent statistical parameters produced during regression in Chapter 4 that indicated multi-proxy training sets performed better than diatom and pollen training sets are not reflected in the RWL reconstruction when the multi-proxy training sets are used to calibrate the fossil assemblages. This indicates that diatom-inferred RWL reconstructions are the most reliable but when diatoms are not present there is the potential to use a multi-proxy approach.

When considering whether local or regional training sets are the most precise, the local diatom, pollen and multi-proxy training sets from Saideal nan Ceapaich in Morar continually provided the most precise estimates of RWL. However, regional training sets provided the most reliable estimates of RWL.

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Chapter 1 Introduction

1.0 INTRODUCTION

Much recent research on relative sea-level (RSL) changes, not just in the UK but numerous locations worldwide (e.g. Zong & Horton, 1999; Horton *et al.*, 1999a, 1999b, 2000, 2006b and 2007; Gehrels, 2000, 2001; Sawai, *et al.*, 2004; Woodroffe, 2006) uses quantitative transfer functions to reconstruct elevation change through sediment sequences. This thesis investigates the success of the transfer function approach using diatom, pollen and multi-proxy training sets taken from NW Scotland. The chapter aims to outline this research project and place it in the broader context of recent sea-level research.

1.1 RESEARCH CONTEXT

The study of relative sea-level (RSL) change has been brought to the forefront of research since questions regarding the importance and potential impact of global warming became an issue. RSL change is a key consequence of climate change over different timescales. The Intergovernmental Panel on Climate Change (2001) stated that global temperature has risen 0.6°C over the last 100 years and that the average sea-level is rising by approximately 1mm yr^{-1}, and the IPCC (2001) have predicted that this figure will increase to >5mm yr^{-1} by 2100. In the UK Climate Change Impacts Programme (UKCIP) Scientific Report (Hulme *et al.*, 2002) future changes in regional net sea-level were calculated for England and Scotland using estimates of present rates of relative land / sea-level changes (isostatic adjustment) using the data of Shennan & Horton (2002). Climate change is a very important topic at the moment and there are concerns regarding impacts such as sea-level rise and coastal erosion. The impacts of climate change could have important implications for the management of our coastlines and how they will look in the future. In turn sea-level rise could have socio-economic implications. For example, in Britain, the 12 429 km of coastline are estimated to yield a total UK annual turnover by the marine related sector of the economy of £80 billion (Turner *et al.*, 1998). The study of past sea-level change is therefore critical if we are to be able to understand, predict and manage future sea-level rise. Studying sea-level change throughout the Holocene helps our understanding of the variability of past sea-level changes and their interaction with climate change and the response of the Earth's crust to changing masses of continental ice and ocean water. Reliable sea-level index points provide a stringent test of models of Glacial Isostatic Adjustment (GIA) (e.g. Lambeck, 1995; Peltier, 1998; Peltier *et al.*, 2002; Shennan *et al.,* 2000; Shennan *et al.*, 2002a; Shennan & Horton, 2002).

Due to its sensitivity to isostatic and eustatic sea-level change the west coast of Scotland has been an important area to study sea-level change. Recently, north west Scotland has been used to refine GIA models because of its occupation by the ice sheets of the last glacial maximum (LGM) and its long record from 16 000 BP to present (e.g. Shennan *et al.*, 2000) as the ice sheets retreated. Very few places in the world provide long, >10 000 yr, records of RSL change, yet they are vital to determining changes in global ice volume. There are several factors that must be taken into consideration when understanding relative sea-level change in this region. In such near field sites there is a complexity of processes occurring following deglaciation, because both land uplift and sea-level rise occur, giving rise to sequences of raised shorelines that reflect the complex interplay between isostatic and eustatic factors. Shennan *et al.* (2000) show that features such as raised tidal marshes and isolation basins in north west Scotland provide well constrained records of changes in relative sea-level following deglaciation during the Late Devensian to present. The Holocene highstand record of the area studied in Scotland is preserved within the many isolation basins and marsh sediments, which collectively preserve a diachronous record of marginal marine sedimentation over the course of the Holocene. Evidence for Late Devensian and Holocene sea-level changes has been examined in the Arisaig area, and this particular region preserves one of the longest records of relative sea-level change in Great Britain, in excess of 16 ka (e.g. Shennan *et al.*, 1993, 1994, 1995a; 1995b).

Change in relative sea level ($\Delta\xi_{rsl}$) at time (τ) and location (φ) can be expressed as:

$$\Delta\xi_{rsl}(\tau,\varphi) = \Delta\xi_{eus}(\tau) + \Delta\xi_{iso}(\tau,\varphi) + \Delta\xi_{tect}(\tau,\varphi) + \Delta\xi_{local}(\tau,\varphi)$$

Where $\Delta\xi_{eus}(\tau)$ is the time dependent eustatic function, $\Delta\xi_{iso}(\tau,\varphi)$ is the isostatic effects of glacial rebound including the contributions of both ice (glacio-isostatic) and water (hydro-isostatic) load contributions, $\Delta\xi_{tect}(\tau,\varphi)$ is any tectonic process, usually considered as negligible in the UK, and $\Delta\xi_{local}(\tau,\varphi)$ which is the total effect of local processes at the site being investigated (Shennan & Horton, 2002).

The research in this thesis is beneficial for the GIA process as transfer functions are capable of reconstructing former sea-levels throughout the whole of a sediment core, as long as the microfossils are preserved and once the samples are dated they could provide a series of sea-level index points to test GIA models.

1.2 RESEARCH AIMS

This thesis investigates Holocene relative sea-level changes using transfer functions in three locations and in combination to form a regional training set for the west coast of Scotland, UK. The main aims are:

1. To develop transfer functions for a regional training set and three local training sets to reconstruct the fossil reference water levels using modern diatom, pollen and combined diatom and pollen (multi-proxy) training sets.
2. To use these transfer functions to provide reconstructions of relative sea-level by applying the modern data to fossil datasets from Nonach, Mointeach Mhor North and Barr-na-Criche.
3. To compare the different microfossil reconstructions and those arising from regional versus site-specific transfer function models.

Broader research questions are:

1. Which transfer function models demonstrate the best performance, diatom, pollen or multi-proxy?
2. When comparing regional versus site-specific transfer function models, which reconstructions, local or regional, provide the most accurate and precise reconstructions?
3. To determine whether multi-proxy transfer functions can reconstruct RWL more precisely and reduce the vertical error bars associated with RWL reconstruction?

1.3 RECONSTRUCTING SEA-LEVEL

1.3.1 Definitions

Elevation refers to a measurement of elevation in meters above Ordnance Datum Newlyn (OD), the UK levelling Datum at Newlyn in Cornwall, south west England.

Mean sea-level refers to the mean sea-level calculated by taking out tidal movement averaged over a period of time, such that periodic changes in sea level (e.g. due to the tides) are also averaged out.

Reference Water Level (RWL) in this study the RWL reconstructions produced show the WA-PLS- or PLS-inferred elevation at which the assemblages occurred relative to the present tidal level. Values of RWL are inferred from the diatom, pollen and multi-proxy transfer functions presented in this thesis.

Mean High Water Spring Tides (MHWS). The height of mean high water spring tides is the average throughout the year of two successive high waters during those periods of 24 hours when the range of the tide is at its greatest.

Mean Tide Level (MTL) is the average of low and high water over a period of time. It varies from place to place and is often used in the construction of sea-level curves.

Highest Astronomical Tide (HAT) is the highest level that can be expected to occur under average meterological conditions and under any combination of astronomical conditions.

Transgression and regression are descriptive terms used in a variety of contexts. In this research the term transgression would be used to describe a change in lithology from a semi-terrestrial to shallow marine deposit, and regression to describe a shallow marine environment replaced by a semi-terrestrial deposit.

Proxy sea-level indicators including landform, sedimentary and fossil data which provides indirect evidence of the position of former sea-levels.

A **sea-level index point** is a data point that when plotted on a graph of relative sea-level over time produces a sea-level curve. Each sea-level index point has an age, elevation, location and tendency. Each sea-level index point also has associated age and elevation errors. Sea-level tendency is defined as positive if the dated sample records an increase in marine influence and is negative if it records a decrease in marine influence (e.g. Tooley, 1978; Shennan *et al.*, 2000). Lithological and bio-stratigraphical data define the palaeo-environment in which the sediment accumulated and the altitude of that palaeo-environment in relation to a fossil tide level.

The **indicative meaning** is the relationship of a proxy indicator to the environment in which it accumulated and its reference water level (Shennan 1980, 1982, 1986; Van de Plassche, 1986). The indicative meaning comprises a reference water level, represented by the dated sample, and an error term, which Shennan (1980) referred to as the 'Indicative Range'.

A **near-field site** is a site that lies in close proximity to the limits of the ice sheets of the last glacial maximum (LGM). Near-fields sites are important due to the complexity of processes occurring following deglaciation, because both land uplift and sea-level rise occur, allowing the study of the complex interplay between isostatic and eustatic factors.

The **mid-Holocene highstand** or mid-Holocene maximum is a period, for example at Arisaig, approximately 7 kyr cal BP in the relative sea-level record when mean RSL peaked. Numerous sea-level index points indicate that the RSL highstand persisted for more than 1000 years before the onset of relative sea-level fall to the present (e.g. Shennan *et al.*, 2005).

1.3.2 Sea-level indicators and techniques

Indicators used for relative sea-level reconstructions in Scotland

There is a wide range of geomorphological evidence for sea-level change in Scotland including landform, sedimentary and fossil data.

Landform data have been used for many years as evidence of relative sea-level changes around the coasts of Scotland (e.g. Smith *et al.*, 1992; Dawson and Smith, 1997). Former coastal landforms that can be used a proxy indicators for former sea levels that now stand above present day sea-level include rock platforms (Wright, 1937), raised beaches (Jamieson, 1865; Wright, 1937; McCann, 1961; Tooley and Smith, 2005), gravel deposits (Wright, 1937), deltas, spits and shingle ridges (King and Wheeler 1963; Sissons, 1962, 1966). Many examples of these features around the Scottish coast are well documented in Steers (1973). The location and elevation of many of these features and the association of these former coastlines with a vertical range of sea-level has been estimated by a number of researchers since the mid-1800s. These often fragmented landform data were then augmented by combining the geomorphological data with the sediment stratigraphy, producing a more continuous record of sea-level change and verifying the origins of sediments by microfossil analysis (e.g. Tooley and Smith, 2005).

More recently littoral sediments have been analysed for their microfossil content and this biological, or bio-stratigraphical evidence, together with the landform and stratigraphic evidence from cores, can be used to reconstruct a sequence of sea-level changes at a particular location in considerable detail (e.g. Smith and Dawson, 1983; Tooley and Shennan, 1987; Edwards and

Horton, 2000; Shennan *et al.*, 2000, 2005, 2006a, 2006b). These relative sea-level observations are only useful if the sediments have not been eroded or transported since they accumulated. The sediments that satisfy this criteria can then be used as sea-level index points by defining four attributes: location, age, altitude and tendency (Shennan and Horton, 2002). When these microfossil data are utilised to reconstruct RSL they can provide information on a diverse range of inter-related processes such as changes in ice sheet extent, crustal movements, coastal evolution and sedimentary processes (e.g. Peltier *et al.*, 2002; Shennan and Horton, 2002 and Shennan *et al.*, 2006a, 2006b) which are vital for environmental scientists, engineers and decision makers alike.

Pollen analysis, or pollen stratigraphy, is undoubtedly the most widely adopted and versatile technique used in environmental reconstructions of environmental change (e.g. Walker *et al.*, 2003; Davis *et al.*, 2003; Birks, 2003). Pollen stratigraphy has been studied as a means of correlating Quaternary stratigraphic units to reconstruct vegetational history (e.g. Birks, 1980; Huntley and Birks, 1983;), palaeo-climatic changes (e.g. Fauquette *et al.*, 1998; Anderson *et al.*, 1998; Tipping, 1991; Huntley, 1992; Emeis and Dawson, 2003; Davis *et al.*, 2003) and sea-level changes (Tooley, 1987a, Shennan *et al.*, 1999; Shennan and Woodroffe, 2003; Shennan *et al.*, 2003; Shennan *et al.*, 2005; Shennan *et al.*, 2006a).

Plant communities have been studied around the coast of the British Isles and botanists have studied the succession of plant communities along the environmental gradient from marine to terrestrial habitats extensively. This means that species that are frequently encountered on salt marshes are widely documented (e.g. Ranwell, 1968; Brereton, 1971; Ranwell, 1972; Adam, 1978; Rodwell, 1997). When used to reconstruct former sea-levels, pollen can be utilised because regressive and transgressive overlaps in the fossil core stratigraphy contain high frequencies of pollen indicative of a salt marsh habitat, so called salt marsh indicators, such as Chenopodiaceae, Aster-type and *Plantago maritima* (Tooley, 1987a). Pollen has been successfully employed in sea-level studies in Scotland (e.g. Shennan and

Woodroffe, 2003; Shennan *et al.*, 2003; Shennan *et al.*, 2005; Shennan *et al.*, 2006a). As a transfer function has not been carried out using pollen from the west coast of Scotland to date, it is expected that where the preservation of other microfossils is poor, or they are absent, the successful application of a pollen-based transfer function would indicate that pollen could provide a viable alternative method for relative sea-level reconstruction.

Diatoms are commonly used in RSL reconstruction as their ecological preferences are well defined and they are abundant in both coastal sediments and freshwater environments (e.g. Hendy, 1964; Denys, 1991/2 and Vos and de Wolf, 1993). Diatoms have been extensively used in sea-level studies around the world as they are usually abundant in coastal sediments, have specific ecological niches and are sensitive to varying environmental factors (e.g. Palmer and Abbott, 1986; Shennan *et al.*, 1994, 1995a, b; Denys and Baeteman, 1995; Shennan *et al.*, 2000, Horton *et al.*, 2006a, 2006b). Analysis and comparison of diatom assemblages from different coastal lithological sequences has shown that diatoms can give a good indication of changes in marine influence due to the fluctuating proportions of polyhalobous (fully marine), mesohalobous (brackish), oligohalobous (brackish-fresh) and halophobous (exclusively fresh) diatom species and can thus indicate marine regressions and transgressions (Haslett, 2002). There are two schools of thought regarding the relationship between diatoms and altitude relative to the tidal frame. The works of Nelson and Kashima (1993), Hemphill-Haley (1996), Shennan *et al.* (1995, 1996), Zong (1997), Zong and Horton (1998) and Gehrels *et al.*, (2001) suggest a strong vertical zonation of diatom species, implying that the environmental variables that determine diatom distribution are associated with tidal submergence, which in turn, is correlated with the altitude of the marsh surface (Zong and Horton, 1999). In contrast, other research has suggested that other environmental variables influence diatom distributions such as level of nutrients and pH (Denys, 1991/2), type of substrate (Chapman, 1941) and water salinity (Juggins, 1992; Vos and de Wolf, 1993), although it is more likely that a suite of abiotic variables related to the amount of tidal submergence and associated changes in the sediment are actually controlling the distribution of diatom assemblages. Diatoms can be prone to dissolution (e.g. Denys, 1991/2; Ryves *et al.*, 2001), but have still proved to be a valuable tool in environmental reconstruction on the NW coast of Scotland (e.g. Shennan *et al.*, 2000; Shennan and Woodroffe, 2003; Shennan *et al.*, 2005, Shennan *et al.*, 2006) and have successfully been used in transfer functions in other areas around the UK (e.g. Juggins, 1992; Zong and Horton, 1999), therefore diatoms have been chosen as a proxy indicator in this investigation.

Foraminifera are also commonly employed in sea-level studies as in recent years the value of contemporary foraminifera as biological indicators of former sea-levels has been appreciated (e.g. Scott and Medioli, 1978; Horton *et al.*, 1999). The well-defined foraminiferal zones that subdivide the marsh increase the vertical resolution of the deposits, providing accurate sea-level indicators (Scott and Medioli, 1978). Therefore once the environmental variables that control the distribution of contemporary foraminifera are established, they can be employed to determine former sea-levels (Thomas and Varekamp, 1991). However, foraminifera also have limitations in their utilisation, for example, foraminifera are prone to dissolution of their calcareous tests in waters under-saturated with calcium carbonate (Haslett, 2002), and it is known that certain benthic foraminifera (and planktonic foraminifera) are more susceptible to dissolution than others (Corliss and Honjo, 1981). Calcareous foraminifera species are also prone to dissolution in environments were the pore water is acidic (e.g. Lloyd *et al.*, 1999). As a result the preservation of foraminifera can be rather unreliable. An additional problem associated with foraminifera is that they are not present in freshwater environments, and therefore they can only be used to represent marine and brackish phases and cannot be used as proxy indicators in freshwater environments (e.g. Lloyd *et al.*, 1999). Similarly studies on the NW of Scotland by Horton *et al.*, (1999) revealed that Kentra Bay had the lowest species diversity of all the study areas, with only four foraminiferal species found > 5 % of the total. The intertidal environment of Kentra Bay is subject to acidic runoff from a raised bog, which enhances the dissolution of calcareous foraminifera. Hence, many species are not preserved in the death assemblage (Green *et al.*, 1993). Therefore foraminifera have been disregarded from this investigation due to their patchy distribution and limited use in areas above the marine limit.

Techniques for reconstructing sea-level changes

Landform data can be used to produce isobase maps (e.g. Smith *et al.*, 2000) using former shoreline data. Isobase maps approximate the spatial pattern of glacio-isostatic rebound, they use data where prominent shorelines of approximately the same age are found in different areas and use this information to produce isobases of areas of similar isostatic uplift in a generalised pattern. The pattern of concentric isobases, reconstructed either manually or by means of trend surface analysis gives a three dimensional image of the deformation of the land surface by the weight of glacier ice (e.g. Firth *et al.*, 1993; Smith *et al.*, 2000), as shown in figure 1.

These isobase maps do however have limitations, the isobases, like other index points, only show uplift relative to present sea-level, rather than absolute land uplift since deglaciation, isobases may not be synchronous, the feature is often not adequately defined with respect to its modern sea level (i.e. the tidal level at which it was formed, therefore its indicative meaning is less certain), not all features have an independent method of dating (Sutherland, 1983) and isobases show only one point in time and do not yield information regarding the rate of RSL change as do microfossil reconstructions. Similarly Lloyd *et al.* (1999) suggested that isobases are limited in explaining the rate, pattern and magnitude of glacio-isostatic uplift if the shoreline is diachronous and no account is taken of the differences in tidal range between sites and changes in tidal range through time.

The second approach utilised to reconstruct past sea-level, which addresses some of the points described above is the production of sea-level index points. For more accurate reconstruction of sea-level and crustal movements it is of paramount importance that field data are collected that can be radiocarbon dated and its altitude measured accurately to Ordnance Datum, and therefore relative to a modern tide level (Shennan *et al.*, 2000; Sutherland, 1983). Each potential sea-level index point is validated biostratigraphically, with an indicative meaning, a reference water level and an indicative range, a sea-level tendency and a calibrated radiocarbon age (Shennan, 1986). Sea-level tendency is defined as positive if the dated sample records an increase in marine influence and is negative if it records a decrease in marine influence (Shennan *et al.*, 2000). Lithological and bio-stratigraphical data define the palaeo-environment in which the sediment accumulated and the altitude of that palaeo-environment in relation to a fossil tide level.

Plotting the sea-level index points against age produces sea-level curves (Figure 1.2). These graphs can then be interpreted to provide information on the earth's response to surface loading, and on ice sheet dimensions and behaviour (Lambeck, 1991a).

Until recently sea-level studies relied upon the identification and analysis of stratigraphic boundaries between terrestrial freshwater sediments and littoral facies and depended on the simple classification of taxa into either freshwater, brackish and marine taxa or into trees, shrubs, herbs and aquatics etc. noting sea-level indicator species, and providing only qualitative estimates of ecological conditions (e.g. Vos and de Wolf, 1988, 1993; Juggins 1992; Zong and Tooley, 1996, Long et al., 1998; Shennan *et al.*, 1993, 1994, 1995a, 1995b, 2005). More recent research (e.g. Zong and Horton, 1998; Gehrels *et al.*, 2001) has provided empirical information, for example, regarding the inter-tidal distributions of diatoms and their relationship with sea-level. These relationships can then be quantified by using transfer functions (e.g. Birks, 1995) that can be used to derive quantitative predictions of tidal-level and Holocene sea-level history from microfossil assemblages.
It has recently been realised that a multi-proxy approach is beneficial for environmental reconstruction. For example, Gehrels *et al.* (2001) have used the multi-proxy approach and concluded that combined training sets are both more accurate and more precise than training sets containing only one micro-organism group. Other authors (e.g. Ridgeway *et al.* 2000; Battarbee, 2000; Walker *et al.*, 2003; Freund *et al.*, 2004) suggest that palaeo-environmental reconstruction is most secure when a number of different, independent, but

complementary techniques are used. Additional benefits of using a multi-proxy approach are that firstly, one can explore quantitatively the precision of the individual microfossils as sea-level indicators; Secondly, one can investigate the indicative meaning of the pollen and diatoms in combination to determine which method provides a more accurate and precise method. Thirdly, one can use the alternative microfossils to complement the data in the absence of one of the proxy-indicators, which in turn allows, or increases the potential to apply, a transfer function through the whole of a sediment sequence (e.g. figure 3). To date, a multi-proxy, diatom- and pollen-based transfer function has not been used to reconstruct RSL on the NW coast of Scotland. The successful application of a multi-proxy transfer function could indicate that diatom- and pollen-based transfer functions can reconstruct RSL more precisely and reduce the vertical error bars associated with RSL reconstruction.

1.3.3 Relative sea-level studies, west coast of Scotland.

A recent development in studies of glacio-isostacy to improve the understanding of relative sea-level change has been the modelling of glacio-isostatic rebound in Scotland and associated sea-level fluctuations (Lambeck, 1995; Lambeck and Purcell, 2001; Shennan *et al.*, 2000, 2001; Dawson *et al.*, 2002; Peltier *et al.*, 2002 and Shennan and Horton, 2002, Shennan *et al.*, 2006a, 2006b). By the production of sea-level curves these models can be interpreted to provide information on the earth's response to surface loading, and on ice sheet dimensions and behaviour (Lambeck, 1991a). Sea-level curves, comprised of sea-level index points, illustrate the relative sea-level change in a particular area. There is broad agreement with the observed and predicted sea-level changes, but significant discrepancies have also been identified often with differences in the magnitude and age of turning points (Shennan *et al.*, 2000) and the age of the rapid Late Devensian relative fall in sea-level. Therefore the collection of data to produce reliable sea-level index points has been an important process to improve the accuracy of model predictions. Over the past decade the increase in the number of researchers studying GIA processes has resulted in the improvement of quantitative GIA models to explain spatial and temporal patterns of RSL change (e.g. Peltier, 1998; Milne *et al.*, 1998, 1999; Mitrovica *et al.*, 2001; Lambeck *et al.*, 2003 and Peltier, 2002). To understand GIA process models Shennan *et al.* (2002) stated it is vital to understand two significant relationships. Firstly, the isostatic component of RSL change in north west Scotland is highly sensitive to shallow earth structure, especially lithospheric thickness and the viscosity of the upper mantle (Shennan *et al.*, 2000). Secondly, this is in contrast to, and independent from, rheological constraints obtained from regions beneath the Fennoscandia and Laurentide ice sheets where RSL changes show a more pronounced sensitivity to deeper earth structure (Peltier, 1998). Some of the models can produce spatially comprehensive predictions of present rates of sea-level change (e.g. Lambeck and Johnson, 1995; Peltier *et al.*, 2002 and Shennan *et al.*, 2002). However, there are still disagreements between model predictions and RSL observations and recent analysis of different GIA models shows this. The ICE-4G (VM2) global model as described by Peltier *et al.* (2002), even without modification, has been shown to fit most of the time-series data in the UK data set rather well, but it estimates RSL below present since the last glacial maximum (LGM) for sites in Britain beyond the LGM ice sheets, or for areas under thin ice. However it was found that the lithospheric thickness, the feature of the radial viscoelastic structure to which the rebound data from Scotland are most , must be reduced to 90km for a best-fit for the Scottish sites. This revised ice model for the British Isles (ICE-4G UK) described in Shennan *et al.* (2002), once modified also produced a good fit with other sets of RSL observations, such as those from the east coast of the USA and numerous Pacific islands (e.g. Peltier *et al.*, 2002 and Shennan *et al.*, 2002). For Scotland the revised ice model for the British Isles (ICE-4G UK) records a non-monotonic pattern of RSL change showing RSL fall ~19 - ~11 kyr BP, a rise to a mid-Holocene highstand, and RSL fall to present (e.g. Figure 2). The RSL observations that record this non-monotonicity provide a crucial constraint for the ICE-4G (VM2) model with a lithosphere of 90km (Peltier *et al.*, 2002). They also showed how timing and magnitude of the rise to the mid-Holocene highstand and the fall to present could quantify a late-Holocene melting history for Antarctica different to that defined in ICE-4G. The predictions of Shennan *et al.* (2000), who use the modified models developed by Lambeck (1995), and those of Peltier *et al.*

(2002) both produce a reasonable fit with RSL observations from Arisaig (Figure 2), but none of the models provides a unique solution that will produce predictions that fit all sites around the UK. Nationally the models underestimate the spread of observations, both for the maximum RSL values, from sites under the thickest ice in Scotland, and for minimum RSL values from sites on the south coast of the UK (Shennan and Horton, 2002).

1.4 SUMMARY

The transfer function methodology is relatively new and will complement the existing data, but, where until recently the data used to reconstruct RSL was sea level index points taken from regressive and/or transgressive contacts, verified by the microfossil data, this investigation aims to reconstruct RSL change through the sediment sequence using diatom, pollen and multi-proxy microfossil-based transfer functions. This is the first time that a pollen and diatom and pollen multi-proxy transfer function have been carried out on the west coast of Scotland.

Chapter 2 Field Sites

2.0 INTRODUCTION

The aim of this chapter is to describe the field sites and studied in this research project. This chapter will describe the field sites, show their location, describe the local habitats and geology and provide information on the predicted tidal ranges for each of the field sites.

2.1 MODERN SAMPLE SITES

The modern field sites along the west coast of Scotland used in the reconstruction are Nonach, Eilean nan Gall and Balmacara in Kintail, Inverness-shire; Saideal nan Ceapaich in Morar; Loch Creran in Appin and Barr-na-Criche in Knapdale on the Argyll coast. Figure 2.1 shows the approximate location of the study areas in which the field sites occur and Table 2.1 shows the predicted tidal ranges for each of the study sites.

2.1.1 Nonach

Nonach is situated at the eastern end of Loch Long to the southwest of Nonach Lodge, adjacent to the village of Killian in Kintail (figure 2.2). The field site is approximately 18km to the east of Kyle of Lochalsh. Loch Alsh lies to the west of the mouth of Loch Long and Loch Duich lies to the southeast. Loch Long attains a depth of 31m near Dornie (Steers, 1973). Loch Long is described by the JNCC (JNCC, 2002) as the second most brackish of the large Scottish sea lochs. The Joint Nature Conservation Committee (JNCC) (JNCC, 2002) designates lochs Duich, Long and Alsh as a Special Area of Conservation (SAC).

Nonach has a variety of habitats. The seaward habitats are typically rocky mud flats with fucoid algae; towards the shore the mudflats become sandier with cobbles, pebbles and boulders. The low marsh is characterised by an extensive area dominated by salt marsh grass (*Pucinellia maritima*), with a dendritic pattern of salt marsh creeks. The mid-marsh is more species diverse with increased numbers of maritime herbaceous plants and additional grasses such as red fescue (*Festuca rubra*) and creeping bent (*Agrostis stolonifera*) and decreasing salt marsh grass. Grasses, sedges, rushes, bryophytes and herbaceous plants dominate the high marsh. The supra tidal area is comprised of a small area of alder carr (*Alnus glutinosa*) which is quickly replaced by an acidic raised bog dominated by sphagnum mosses (*Sphagnum spp.*) and common heather / Ling (*Calluna vulgaris*). The location of the sample transect at Nonach is shown in figure 2.3.

Nonach lies within the Northern Highlands geological area. This area lies to the south of the Moine Thrust and to the north and west of the Great Glen Fault. The metamorphic rocks of the Northern Highlands are the Moine schists. They were originally deposited as a thick sequence of sandy sediments in a shallow sea 1000 – 850 million years ago and are named after the boggy headland in northern Sutherland known as A'Moine, the Gaelic word for peat (Gillen, 2003). The Monian rocks are characterised by metamorphic schists with granite intrusions (Gillen 2003, Peach & Horne 1930). The Moine is sub-divided into three groups from the oldest in the west to the youngest in the east; these are the Morar, Glenfinnan and Loch Eil groups respectively (Gillen, 2003).

The tidal prediction in the Admiralty Tide Tables (1986) nearest to Nonach is site called Dornie Bridge. The tidal predictions for Dornie Bridge have then been transformed into m OD (Table 2.1). At Dornie Bridge the Mean High Water Spring Tide (MHWST) is 2.62 m OD and Mean Low Water Spring Tide (MLWST) –1.98 m OD.

2.1.2 Eilean nan Gall

Eilean nan Gall is a small rocky promontory on the southern shore of Loch Duich, approximately 2km northeast of Shiel Bridge, near to the village of Invershiel (figure 2.2).

Eilean nan Gall (Plate 2.1) is characterised by a rocky foreshore consisting of coarse sandy flats with abundant cobbles, boulders and fucoid algae. The low marsh is typically dominant by salt marsh grass (*Pucinellia maritima*) and sea thrift (*Armeria maritima*) in the thin turf overlying the very rocky substrate. The mid marsh is more species diverse with increased numbers of maritime herbaceous plants including sea thrift (*A. maritima*) and sea milkwort (*Glaux maritima*) and additional grasses such as red fescue (*Festuca rubra*) and creeping bent (*Agrostis stolonifera*) and increasing sphagnum mosses and other bryophytes and decreasing salt marsh grass. The high marsh is an acid bog habitat dominated by sphagnum mosses (*Sphagnum spp.*) and other bryophytes, for example, *Polytrichum commune*, and soft rush (*Juncus effuses*) and common heather (*Calluna vulgaris*). The supra tidal area is comprised of an area of acidic calluna heath overlying a rocky outcrop with thin soils on the highest part of the Eilean nan Gall promontory. Figure 2.4 shows the location of the sample transect.

Eilean nan Gall lies within the Northern Highlands geological area and its geology is also dominated by Moinian metamorphic rock (Gillen, 2003).

As at Nonach, the nearest location to Eilean nan Gall with a tidal prediction is Dornie Bridge (Table 2.1).

2.1.3 Balmacara

The field site lies on the northern bank of Loch Alsh in Balmacara Bay south of the village of Balmacara and is approximately 6km east of Kyle of Lochalsh (figure 2.2) in Kintail, Inverness-shire.

Balmacara is a small tidal marsh with a restricted number of habitats. The shores of the Loch are characterised by rocky beaches with pebbles, gravel and sand and occasional fucoid algae. The low marsh is not dominated by saltmarsh grass and consists of other grasses and maritime herbs such a sea thrift (*Armeria maritima*) and sea milkwort (*Glaux maritima*). The mid marsh is dominated by red fescue (*Festuca rubra*), creeping bent (*Agrostis stolonifera*, and herbaceous maritime plants, for example, bucks-horn plantain (*Plantago coronopus*) and other herbaceous species, such as broad-leaved dock (*Rumex obtusifolius*). The high marsh is comprised of an area of semi-improved grassland adjacent to a stream lined with sparse wet woodland of alder carr (*Alnus glutinosa*). Figure 2.5 shows the location of the sample transect.

Balmacara lies in the Northwest Highlands geological region. The northwest highlands along with the Outer Hebrides are comprised of some of the oldest rocks in Europe at 3 billion years old. These rocks are known as Lewisian Gneiss Complex after the Isle of Lewis, and are almost exclusively found to the west of the Moine Thrust zone (Gillen, 2003). The Lewisian Gneiss Complex represents a fragment of deep level continental crust belonging to Laurentia. The Torridian sandstone comprises 2000m of river-borne sediments and wind-borne sands of the Stoer group that were deposited directly onto the Lewisian Gneiss in desert conditions, with pebbles and boulders of Lewisian Gneiss found at the base of the Stoer Group (Gillen, 2003). Above the coarse material river-lain sandstones occur, as do shales and a volcanic unit. Lying on top of the Stoer Group is the younger Torridon Group, which is a layer of reddish brown sandstone responsible for the spectacular scenery of the northwest seaboard (Gillen, 2003). Balmacara lies on an area of Torridonian sandstone overlying the Lewisian gneiss (Peach & Horne, 1930; Gillen, 2003).

The coastline here typifies the dominant features of the Lewisian rock, block-folds, shear belts, basic dykes and granite sheets run in a northwest-southeast direction and these features have been accentuated by erosion and the coastline has fjords and sea lochs aligned in this directional trend (Gillen, 2003).

The nearest location to Balmacara with a tidal prediction is Kyle of Lochalsh. At Kyle of Lochalsh the MHWST is 2.57 m OD and the MLWST –1.93 m OD (Table 2.1).

2.1.4 Saideal nan Ceapaich

Saideal nan Ceapaich lies approximately 0.2km north of the village of Arisaig in south Morar (figure 2.6). The study area consists of Saideal nan Ceapaich tidal marsh on the banks of Loch nan Ceall between the Sound of Arisaig to the south and the Sound of Sleat to the north.

The loch edge is characterised by a rocky beach of pebbles, gravel and coarse sand with occasional fucoid algae. The low marsh is dominated by salt marsh grass (*Pucinellia maritima*), maritime herbs such as sea aster (*Aster tripolium*), sea thrift (*Armeria maritima*) and milkwort (*Glaux maritima*). The mid marsh is characterised by salt marsh grass, red fescue (*Festuca rubra*), creeping bent (*Agrostis stonolifera*), scurvy grass (*Cochlearia officinalis*), yarrow (*Achillea millefolium*) and patches of reed (*Phragmites communis*) and soft rush (*Juncus effusus*). The high marsh is dominated by reed (*Phragmites communis*), marsh marigold (*Caltha palustris*), meadowsweet (*Filipendula ulmaria*), soft rush (*Juncus effusus*), broad-leaved dock (*Rumex obtusifolius*), creeping buttercup (*Ranunculus repens*) and occasional yellow-flag (*Iris pseudacorus*). The supra tidal area is characterised by yellow-flag (*I. pseudacorus*), meadowsweet (*F. ulmaria*), soft rush (*J. effusus*), bramble (*Rubus fruticosus*), hawthorn (*Crataegus monogyna*) and grasses such as red fescue (*F. rubra*) and creeping bent (*A. stolonifera*). Figure 2.7 shows the location of the sample transect at Saideal nan Ceapaich.

Saideal nan Ceapaich lies within the Northern Highlands geological region. The geology is dominated by Moinian schists (Gillen, 2003). The coastline in this area is broken and picturesque and relatively low with mainly pale calcareous sand. The coast of the Sound of Arisaig is much indented with numerous small headlands and minor bays (Steers, 1973).

The nearest location to Saideal nan Ceapaich with a tidal prediction is the port of Mallaig to the North. At Mallaig the MHWST is 2.38 m OD and the MLWST –1.92 m OD (Table 2.1).

2.1.5 Loch Creran

Loch Creran is located approximately 15km north east of Oban in Appin on the Argyll coast. Loch Creran is an enclosed marine inlet on the southern shore of Loch Linnhe adjacent to the Lynn of Lorne (Figure 2.8). The study area consists of an area of mud and sand flats and tidal marsh at the mouth of the River Creran that drains Glen Creran. Loch Creran is designated as a Special Area of Conservation (SAC) by the JNCC (JNCC, 2002). This designation is due to an area of biogenic reefs of the calcareous tube-worm *Serpula vermicularis*, the only such reef in the UK.

Loch Creran has a variety of habitats; the shore of the Loch is typically a rocky, pebbly sand flat. The low marsh area is characteristically a grassy sward dominated by salt marsh grass (*Pucinellia maritima*), sea thrift (*Armeria maritima*) and sea milkwort (*Glaux maritima*). The mid marsh is more species diverse with decreasing salt marsh grass (*P. maritima*), increasing red fescue (Festuca rubra) and creeping bent (*Agrostis stolonifera*) and more maritime taxa, for example, sea thrift (*Armeria maritima*), sea milkwort (*Glaux maritima*), scurvy grass (*Cochlearia officinalis*) and patches of soft rush (*Juncus effusus*). The high marsh has a more acidic bog community with soft rush (*J. effuses*), sphagnum mosses (*Sphagnum spp.*), bryophytes, sedges and common heather (*C. vulgaris*) dominating. The supra tidal area is a small stand of alder carr (*Alnus glutinosa*) within the bog characterised by abundant sphagnum mosses (*Sphagnum spp*), soft rush (*J. effuses*), bryophytes (e.g. *Polytrichum commune*) and sedges. Figure 2.9 and Plate 2.2 show the location of the sample transect.

Loch Creran lies within the Grampian Highlands geological region. Argyll consists of a base of Dalradian metamorphic rock (Gillen, 2003), Dalradian is the term used for the rocks south of the great Glen Fault (Geike, 1897). Dalradian metamorphic rock resembles the older Moine rocks in many ways, but at 25km in depth is much thicker and more varied, especially in the upper units (Gillen, 2003). In addition to schists and quartzites, there are also limestones, slates, phyllites, grits and volcanic rocks, as well as glacial deposits (Gillen, 2003). Highly complex folded and metamorphosed rocks dominate the Grampian Highlands. Geographically and geologically the Grampian Highlands are very complex, and is sub-divided into several areas. The area comprising the southwest Highlands in Argyll is typically Dalradian schist overlain by younger (Devonian) lavas of Lorne and intruded by the tertiary igneous complex of Glencoe (Gillen, 2003; Sissons, 1967).

The nearest location to Loch Creran with a tidal prediction is Port Appin to the north. At Port Appin the MHWST is 2.25 m OD and the MLWST –1.15 m OD (Table 2.1).

2.1.6 Barr-na-Criche

Barr-na-Criche lies on the northern shore of West Loch Tarbert in Knapdale on the Argyll coast (figure 2.10). The study area consists of Achadh-Chaorann Bay and the raised marsh approximately 0.4km south west of the hamlet of Barr-na-Criche. The marsh at Barr-na-Criche is part of an extensive area of raised marsh that stretches in excess of 3 km inland in a northeasterly direction past the village of Clachaig. The main stream that drains into Achadh-Chaorann Bay arises at Lochan na Moine-cioba, and its tributaries drain the surrounding hills.

Figure 2.11 shows that the sample transect begins on the mudflats at the south of the stream and is orientated in a north-westerly direction to the east of Muir Achaid and up to the higher ground on the slopes of Barr a' Mhuilinn.

At low tide Achadh-Chaorann Bay has a large expanse of exposed mudflats. A narrow band of low marsh dominated by salt marsh grass (*Pucinellia maritima*) and sea thrift (*Armeria maritima*) occurs around the edges of the bay. Landward of the low marsh is an extensive area of raised tidal marsh This extensive area of mid marsh is a mosaic of vegetation with occasional creeks and a stream which drains the surrounding area. The mid marsh is dominated by a variety of grasses, bryophytes, sedges and rushes with large stands of soft rush (*Juncus effuses*) in wetter areas and drier hummocks have a variety of bryophytes, sedges and bog myrtle (*Myrica gale*). The high marsh is typically acidic bog dominated by *Sphagnum spp.*, bryophytes, for example, *Polythricum commune*, and common heather (*Calluna vulgaris*) and bog myrtle (*Myrica gale*). Drier areas on the rocky slopes of Barr a' Mhuilinn have abundant common heather (*C. vulgaris*) and bog myrtle (*M. gale*), bryophytes and lichens. Figure 2.11 and Plate 2.3 show the location of the sample transect.

Barr-na-Criche lies within the Grampian Highlands geological region; this area of the southwest Highlands in Argyll is typically dominated by Dalradian metamorphic rocks (Gillen, 2003; Peach & Horne, 1930).

The nearest location to Barr-na-Criche with a tidal prediction is East Loch Tarbert. At East Loch Tarbert MHWST is 1.78 m OD and MLWST −1.32 m OD (Table 2.1).

2.2 FOSSIL SAMPLE SITES

Three fossil samples have been utilised to allow the reconstruction of former sea-levels. A fossil core is being used from Kintail, Morar and Knapdale to reconstruct former sea-levels.

2.2.1 Nonach

Core NN04 is taken from Kintail, Inverness-shire. The core sampled for microfossil analysis at Nonach was taken from an area of calluna mire to the north of the modern sample transect taken on the marsh. The fossil core sample site is situated to the east of a fork in the road where a private road leads northeast to Nonach Lodge (figure 2.12). The elevation of core NN04 (3.97 m OD) and a brief description of the litho-stratigraphy are listed in Appendix 5.1.

2.2.2 Mointeach Mhor North

Two monolith samples from Mointeach Mhor North in Morar (MMN01A and MMN01B) have both been utilised to provide a microfossil record from Morar (MMN01A&B). The monolith samples were taken from Mointeach Mhor North in 2001 for use in additional studies (Shennan *et al.*, 2005). The series of monolith samples and cores were taken from a fossil sand dune system at the west of Mointeach Mhor North in a transect moving landward. Monoliths A and B were taken from the landward side of the fossil sand dune (figure 2.13).

The elevation of monolith MMN01A & B (9.37 m OD) and a brief description of the litho-stratigraphy is listed in Appendix 5.1.

2.2.3 Barr-na-Criche

Core BC006a is one of a series of 22 cores taken from Barr-na-Criche, Knapdale on the Argyll coast. Core BC006a is taken from the raised marsh to the east of Muir Achaidh (figure 2.14). Some cores from the series of cores taken from Barr-na-Criche have recently been published in other studies (Shennan *et al.*, 2006a). The elevation of core BC006a (3.34 m OD) and a brief description of the litho-stratigraphy are listed in Appendix 5.1.

2.3 SUMMARY

This chapter shows the location of the modern and fossil sample sites and describes the habitats, geology and tidal regime in each area under investigation. The modern samples taken from the six field sites described above allow me achieve the aims and answer the broader research questions in Chapter 1 as they allow comparison of site-specific (or local) versus regional reference water level reconstructions for diatom, pollen and multi-proxy microfossil reconstructions when applied to the fossil cores. The location and elevation of the fossil cores that are going to be used for the reference water level reconstructions are also provided.

Chapter 3 Methodology

3.1 INTRODUCTION

The aims of this chapter are to outline the methods used and to explain why each method is considered appropriate. Techniques discussed include the sampling methodologies of the modern samples and fossil cores, preparation of the pollen and diatom samples, their subsequent analysis, selection of environmental variables and their laboratory preparation; and finally the statistical methods.

3.2 COLLECTION OF MODERN SURFACE SAMPLES

3.2.1 Selection of modern study sites

Six modern sample sites were chosen from tidal marshes with a variety of habitats along an environmental gradient from fully marine to freshwater environments in close proximity to the fossil sample sites previously sampled in Shennan *et al.*, 2005, 2006a. It is important that the modern marshes represent a range and variety of habitats comparable to those in the fossil cores. The quality of the marshes was evaluated with regard to their ecology, species diversity and anthropogenic impact. The sites have been visually assessed for suitability on previous field visits, noting the grazing regime, size, and habitat types present. Scott (1984) stated that there are many good quality or Grade A salt marshes in the area. Modern sample sites were selected which have high species diversity, show good vegetational succession and are as natural as possible and therefore are as similar as possible to salt marshes that may have occurred naturally throughout the Holocene. Anthropogenic factors that could render the marshes unsuitable include intensive grazing, peat cutting and artificial features associated with land reclamation.

3.2.2 Sampling methodology

The first step was to review the fossil data. This was particularly useful when considering the fossil pollen data. The modern sample sites could then incorporate habitat types that were known to be represented in the fossil cores e.g. alder carr, Sphagnum bog and Calluna mire in addition to salt marsh habitats. This then decreases the chance of non-analogues when comparing the modern and fossil data. This was not applicable to the fossil diatom assemblages which could not be assessed by visual reconnaissance, therefore modern microfossil samples were taken from transects encompassing an environmental gradient that contained as many microhabitats and assemblage types as possible to reduce the occasions whereby a fossil assemblage is not represented in the modern samples. Preliminary statistical analyses were carried out to determine whether there were any inadequacies in the data and whether any further samples were required to improve the performance and therefore precision of the transfer functions.

For each modern field site, sample stations were selected along a transect within the inter-tidal zone (the number of samples was determined by the vertical range of the inter-tidal area). Transects were arranged to incorporate a range of environments from above Highest Astronomical Tide (HAT), and as near to Lowest Astronomical Tide (LAT) as possible, taking in sub-tidal areas where feasible. Samples were taken closer together across transitional environments, for example, across the transition between mud flat and low marsh or high marsh and acidic bog to ensure a variety of transitional microhabitats were sampled.

3.2.3 Elevation

Each fossil core and each modern sample was instrumentally levelled to a local Ordnance Datum (OD) benchmark or previously levelled temporary benchmark (TBM) using a Leica TC 1010 total station.

3.3 COLLECTION OF FOSSIL SAMPLES

3.3.1 Selection of fossil cores

From a selection of fossil cores taken by Shennan (Shennan *et al.*, 2005, 2006a) fossil samples were chosen that represented a variety of palaeo-habitats/environments that have occurred throughout the Holocene to provide as many fossil analogues as possible to which the transfer function technique can be applied.

The fossil samples comprise a piston core sample collected from Nonach in Kintail, monolith samples from Mointeach Mhor North, Morar and a 25 mm diameter gouge core sample from Barr-na-Criche, Knapdale.

3.3.2 Origin of fossil samples

The fossil samples used in this research were collected by Prof. Shennan and myself between the years 2000 and 2005 in my capacity as a Research Associate. The subsequent diatom and pollen analysis of various cores samples taken from the west coast of Scotland was undertaken by me and it was therefore agreed that these cores could be used in this research as a different methodology (transfer functions) was being used to reconstruct former sea-levels. There was a choice of many cores and monolith samples from the Arisaig area (Morar) and Knapdale. This meant that although the choice of where the fossil samples originated from was not optional, it was possible to collect additional modern samples by returning to the field sites where fossil samples were previously taken. This allowed me to create local training sets that could be combined with the other modern samples to create a regional training set to allow both local and regional comparisons. For this research a fossil core sample collected from Nonach in Kintail, and three transects of modern samples from Balmacara, Nonach and Eilean nan Gall were collected, resulting in a fossil core and modern samples from further north. The benefit of having multiple locations over tens to hundreds of kilometres apart is apparent for comparisons of observations with predictions from models of glacial isostatic adjustment to evaluate sensitivity to different model parameters (Peltier *et al.*, 2002; Shennan *et al.*, 2000) should these samples be used in further research to test GIA models.

Mointeach Mhor North, one of the fossil sites in this investigation, is an important site on the north west coast because it records both the rise and fall of sea level throughout the mid Holocene highstand (e.g. Shennan *et al.* 2005) more precisely than other sites. The existing sea-level index points provide data on the timing and height of the rise and fall of sea level during the mid-Holocene highstand, but using the previously analysed microfossil data a transfer function can be applied to the microfossil data to reconstruct RSL change through the whole of the sediment sequence, including the peak of marine influence in the sediment in between the sea level index points (Figure 3). Although a calibrated radiocarbon date is not assigned to each sample showing the dates of RSL change the magnitude of change can be reconstructed and the samples could be dated in future to produce a suite of sea-level index points and used, for example, to test GIA models.

3.3.3 Sampling methodology

Depending on the sediment types fossil samples were taken using either a 25 mm diameter gouge core, Russian corer or 50 mm piston corer. Several samples were taken in monolith tins from Mointeach Mhor North. All samples were placed in protective plastic tubing and wrapped in polyethene and refrigerated below 4°C to prevent oxidation and microbial activity. The exposed sediment sample was cleaned with a knife to produce a smooth surface and so helped reduce the risk of contamination.

Samples were taken from areas where sedimentation was continuous and where there appeared to be no hiatus in the sequence, for example, samples would not be taken from areas where peat cutting was evident.

For each fossil sample the litho-stratigraphy was recorded following the methodology of Troels-Smith (1955). Microfossil samples were taken from the fossil cores at intervals of between 1 - 5 cm. More regular sampling (1 - 2 cm) was undertaken across changes in the lithology that had the potential to yield bio-stratigraphical evidence of relative sea-level (RSL) change.

3.4 COLLECTION OF ENVIRONMENTAL SAMPLES

3.4.1 Sampling methodology

A sample of sediment ~ 30 cm^3 (30 cm^2 by 1 cm thick) was taken for analysis of environmental variables. The samples were cut from the marsh surface with a knife and placed in sealed plastic bags for storage and refrigerated below 4°C to prevent oxidation and microbial activity.

3.4.2 Selection of environmental variables

Several environmental variables are investigated that are thought to influence the spatial distribution of species in natural communities. The zonation of diatom assemblages across steep environmental gradients is explained by two differing mechanisms. Research by Nelson and Kashima (1993), Hemphill-Haley (1996), Shennan *et al.* (1995,1996), Zong and Horton (1998) and Horton (1998) suggest a strong vertical zonation of diatom species and implies that all the environmental variables that determine diatom distribution are related to tidal submergence, which in turn is correlated with altitude of the marsh surface. Other research has inferred that additional environmental variables also influences the spatial distribution of diatoms including level of nutrients (Denys, 1991-2), pH (Denys, 1991-2; Gasse *et al.*, 1995; Barker *et al.*, 2002), type of substrate (Chapman, 1941; Sawai, *et al.*, 2004), water salinity (Hudsted, 1957; Fritz, 1990; Juggins 1992; Vos & de Wolf, 1993; Gasse, *et al.* 1995; Gasse, *et al.* 1997; Sherrod, 1999; Roberts, *et al.*, 1999; Gasse, 2002; Sawai *et al.*, 2004), loss on ignition (Sawai *et al.*, 2004), soil moisture (Harrison *et al.*, 1998; Battarbee, 2000) and water depth (Campeau *et al*,. 1999). The environmental factors examined have been recognised as important variables affecting the distribution and abundance of modern plant species. Previous research carried out by Hillier (2000) indicated that elevation, salinity, pH, LOI and the percentage of sand, silt and clay were the most important factors affecting the distribution of modern diatom assemblages.

Research suggests that the environmental factors that influence the spatial distribution of salt marsh plants is generally as a result of community composition shifts along a salinity gradient (Ungar, 1967; Bertness *et al.*, 1992; Pennings and Callaway, 1992; Pennings *et al.*, 2003; Crain *et al.*, 2004) in relation to elevation of the marsh surface (Morris *et al.*, 2002). Alternatively some research suggests that competition for nutrients may also influence the spatial distribution of plant species (Smart and Barko, 1980; Emery *et al.*, 2001).

The environmental variables being investigated are elevation converted into Standardised Water Level Index (SWLI), salinity, loss on ignition, pH and sediment grain size. These environmental variables have been chosen as they have proved to be important environmental variables that influence the spatial distribution of diatom species and plant species, and thus pollen.

Due to time constraints not all of the environmental variables were analysed for each sample. The full modern sample set (training set), consisting of 116 samples, has associated elevation (m OD) and Standardised Water Level Index (SWLI) data. However only 74 samples from Saideal nan Ceapaich, Barr-na-Criche and Loch Creran also have associated salinity, LOI, pH and sediment grain size (% sand, % silt & % clay) data in addition to the elevation and SWLI data to produce the modern training set.

3.5 LABORATORY METHODS

3.5.1 Loss on ignition

The organic content of the samples is calculated using the loss on ignition method following the methodology of Ball (1964).

Approximately 5g of sediment is weighed accurately into a weighed crucible. The sample is left to oven dry overnight at 105°C then the crucible and sample are re-weighed. The crucible and sample are then placed in a muffle furnace preheated to 550°C for 5 hours. The sample is then removed from the furnace allowed to cool in a dessicator and re-weighed. The following equation is used to calculate the loss on ignition:

$$\textbf{Loss on ignition (\%)} = \mathbf{(F - G)/(F - E) \times 100}$$

Where E = weight of crucible, F= weight of crucible and oven dry soil and G= weight of crucible and ignited soil.

3.5.2 Sediment grain size

Sediment grain size was measured using a Coulter laser particle size granulometer. Approximately 0.5 g of sediment was placed in a 50 ml sample tube. 10 ml of distilled water is added, washing the sediment to the bottom of the tube and placed in a rack. 10 ml of 20% hydrogen peroxide is then added. The sample tubes were then covered with aluminium foil and placed in a boiling water bath for 2-4 hours. If any organic material was still present more hydrogen peroxide was added and the tubes placed in the water bath for a further 2 hours. This was repeated until all the organic material had been dissolved. The samples were then centrifuged at 4000 rpm for 4 minutes, half of the supernatant decanted off, topped up with distilled water, centrifuged and decanted again. 20 ml of distilled water and 2 ml of sodium hexametaphosphate solution was then added. The samples were then ready to be analysed in the Coulter granulometer. After being analysed the sand, silt and clay fractions are classified according to the Wentworth Scale (Wentworth, 1922).

A Coulter laser particle size granulometer can only measure sediments with a grain size of less than 2 mm. The tidal flats often consisted of coarse sediments, for example, coarse sand often with pebbles, cobbles and boulders. In these circumstances samples were taken from the same environment as the diatom and pollen samples were taken to allow direct comparison, therefore finer grained sediments (clay, silt, sand, gravel and small pebbles) were taken for laboratory analysis and notes made of the types of sediment characteristic of the habitat.

3.5.3 pH

A calibrated Jenway 3320 pH meter was used to measure pH. Approximately 20 g of sediment was placed in a beaker with an equal amount of distilled water and made into a thin paste. After being left to stand for one hour to allow the sediment to disaggregate the probe was placed into the paste and the pH value recorded. To prevent contamination the electrode was washed with distilled water between samples.

3.5.4 Salinity

Conductivity was measured in microsiemens (μs cm^{-1}) or millisiemens (ms cm^{-1}) where appropriate, using either a Jenway 4320 conductivity meter or a EIL 5003 conductivity meter MC-MK V when the conductivity was very low. Laboratory tests showed that this equipment was more accurate at low conductivities but at higher conductivities (>0.4 ms cm^{-1}) were comparable to the results of the Jenway 4320. The salinity in gL^{-1} was then calculated using the following simple conversion:

$$\textbf{Salinity (gL}^{-1}\textbf{) = 0.851 x conductivity (ms cm}^{-1}\textbf{) – 1.373}$$

3.5.5 Standardised Water Level Index (SWLI)

All tidal information and predictions are from the locally published Admiralty Tide Tables (UK Hydrographic Office, 1986).

The most important, or predictor variable in the modern training set is elevation (m OD). To allow comparison between samples from different geological locations with differing tidal characteristics the elevation of each sample (m OD) is then converted into Standardised Water Level Index (SWLI) using a simple equation to calculate the relationship between the modern sample elevation (m OD) and MHWS at the location of the nearest tidal prediction (Table 2.1)

Standardised water level index is calculated by using the following equation after Horton (1997):

$$\text{SWLI} = \quad [((\text{Sample altitude m OD} - \text{MTL tidal station}) / (\text{MHWS tidal station m OD} - \text{MTL tidal station m OD}) \times 100) + 100]$$

SWLI therefore allows comparison between all of the samples when combining samples to create a large training set.

3.6 MICROFOSSIL ANALYSIS

3.6.1 Sampling methodology

Surface samples were collected from each sample station for microfossil analysis of a standardised volume of ~10 cm^3 (10 cm^2 by 1 cm thick). Microfossil surface samples were stored in sealed bags and refrigerated below 4°C to prevent oxidation and microbial activity.

3.6.2 The halobian classification system

A major control on the distribution of diatom species is salinity. The system used to classify diatoms according to their salinity tolerance is called the halobian system of classification. This system was first devised by Kolbe (1927) and has been subsequently modified by Hudstedt (1953; 1957) and Hemphill-Haley (1993) amongst others. The halobian system of classification has four main groups, an explanation of which is shown in table 3.1.

Table 3.1 The halobian classification system (Hemphill-Haley, 1993)

Classification	Salinity range (‰)	Description
Polyhalobous	>30	Marine
Mesohalobous	0.2 to 30	Brackish
Oligohalobous-halophile	<0.2	Freshwater – stimulated at low salinity
Oligohalobous-indifferent	<0.2	Freshwater – tolerates low salinity
Halophobous	0	Salt-intolerant

A basic interpretation of this classification system should see a change in the salinity classes of the diatom assemblages as one moves from the tidal flat through the salt marsh and into the freshwater environments above the HAT. As one would expect, polyhalobous species occur in sub-tidal areas and on the tidal flat along with mesohalobous diatom species. As marine influence decreases oligohalobous-halophilous and oligohalobous-indifferent species will increase as polyhalobous and mesohalobous species decrease. Finally halophobous species will occur above the HAT in the freshwater environments.

Diatom assemblages from coastal depositional environments have high species diversity, with each habitat type potentially having a distinct diatom community. The fossil diatom communities from coastal environments can therefore provide a reliable record of environmental change (Haslett, 2002). The halobian classification can be utilised in the production of percentage abundance diagrams as a simple visual aid that shows a basic summary of the marine influence (or salinity tolerance) for each diatom assemblage for both modern surface samples and fossil cores (e.g. Shennan *et al.* 1994).

3.6.3 Diatom preparation

Diatom samples were prepared for investigation with a light microscope following the standard methodology of Palmer and Abbott (1986). Approximately 0.5 cm^3 of sediment was taken from each modern sediment sample or sample depth of the fossil core. These were then digested in 70-100 ml of 20% H_2O_2 by heating gently in a water bath for up to 24 hours, or until all organic matter was removed from the sample. If the samples had a very high organic content after 24 hours the samples were centrifuged, the supernatant decanted and 70-100 ml of fresh H_2O_2 added and the process repeated. Two and five drops of digested sample were pipetted onto two cover slips with 10 drops of distilled water and dried on a warm hotplate. The cover slips (a) and (b) of differing concentration were then inverted and placed onto a glass slide, using Zrax, a high refractive index medium mountant with a refractive index of 1.7+. The glass slides were then heated at 100°C until the Zrax no longer bubbled and the slide allowed to cool and the mountant to set.

3.6.4 Pollen classification

The pollen is simply classified into life form of the plant from which it originated. The life form indicates changes in the community structure of the vegetation and assists in determining habitat change. For example, the life form classification will illustrate changes in vegetation from calluna mire dominated by grasses and shrubs to a wet woodland environment dominated by tree pollen. The pollen grains are defined as tree, shrub, herbaceous plant or aquatic plant. Additional classifications include spores (for example mosses and ferns), and other, including dinoflagellates, pediastrum and foram test linings, all of which are sometimes encountered in the prepared pollen slides. The life form of the plants from which the pollen or spores originated can be determined by using any good book on British flora (e.g. Keble, 1965). To aid in the interpretation of pollen diagrams indicator species commonly found on salt marshes such as *Plantago maritima* can be highlighted.

3.6.4 Pollen preparation

Pollen samples were prepared for investigation with a light microscope following the standard methodology of Moore *et al.* (1981). The laboratory procedure for pollen analysis involves five steps.

The first step, the evacuation of alkali soluble organic compounds involves adding ~20 ml potassium hydroxide to 1.0 cm^3 of sample in a plastic test tube, and heating in boiling water for 30 minutes stirring occasionally. The mixture is then decanted through a 180 micron sieve, the residue washed with distilled water and centrifuged at 4000 rpm for 4 minutes. The sample is then decanted and washed until the supernatant is unstained.
Step 2 is the hydroflouric digestion of siliceous material. Hydrofluoric acid is added and the sample is heated in boiling water until the sediment dispenses and stratified sediment appears (~ 1 hour). The sample is then stirred, centrifuged and the supernatant decanted. Hydrochloric acid (10% solution) is then added and this is heated in boiling water for 3-5 minutes, centrifuged, decanted and washed with distilled water, then stirred, centrifuged and the supernatant decanted. This is transferred into narrow plastic test tubes.

Step 3 is the evacuation of unaltered lignin and cellulose. Approximately 20 ml of glacial acetic acid is added, the mixture is then stirred, centrifuged and the supernatant decanted. Then approximately 20 ml of acetylation mixture (1:9 conc. Sulphuric acid – acetic anhydride) is added and stirred well. This is then heated in boiling water for one minute then topped up with glacial acetic acid, centrifuged and the supernatant decanted. Glacial acetic acid is then added, stirred, centrifuged then the supernatant decanted. Distilled water is then added and the mixture stirred, centrifuged and the decanted twice.

The fourth step is staining the pollen. The sample is washed with ethanol twice to remove water, ensuring the test tube walls are rinsed, then centrifuged and the supernatant decanted. Two ml of tertiary Butyl Alcohol and two drops of safranin is added then the sample is transferred into small glass sample vials, centrifuged and decanted. Silicone fluid at approximately the same volume as sample is added and the mixture is stirred and cotton wool is used to plug the vial. The vials are then left for several hours until the remaining tertiary butyl alcohol evaporates.

The final step is making the pollen slides for microscopial examination. Several drops of silicon fluid are dropped onto a microscope slide. A wooden stirrer is then used to thoroughly mix the sample in the vial, and then a small amount of sample is extracted on the stirrer and mixed into the silicon fluid on the microscope slide. Finally a 22 x 44 mm coverslip is placed onto the microscope slide. The sample is now ready for pollen analysis.

3.6.6 Microfossil sample counts

After the pollen and diatom slides are prepared a minimum count of between 200-250 microfossils are counted from each sample (following Shennan *et al.* 1995; Campeau *et al.*, 1999; Plater & Shennan, 1992; Evans *et al.*, 2001; Freund *et al.*, 2004; Hamilton *et al.*, 2005). Diatoms were identified at a magnification of 1000 times using the keys of Van der Werff and Huls (1958-74) and additional texts (Kelly, 2000; Barber *et al.*, 1981) were used to cross reference freshwater taxa. Pollen was identified at a magnification of either 600 or 1000 times depending on the appropriate magnification required for identification using the keys of Moore and Webb (1978) and Moore *et al.* (1991).

The main challenge in marine research is the problem in distinguishing between autochthonous and transported, allochthonous species in tidal and estuarine environments (Simonsen, 1962). Various studies have attempted to understand the taphonomy of pollen (e.g. Mudie *et al.*, 1994; Chmura *et al.*, 1995; Freund *et al.*, 2004) and diatom assemblages (thanatocoenoses) (e.g. Sherrod *et al.*, 1989; Denys, 1994; Zong, 1997; Zong and Horton, 1999 and Sawai, 2001b). Zong and Horton (1999) state that in relatively high energy environments such as tidal marshes, the surface diatom assemblages collected at each sampling station are likely to be a mixture of locally produced taxa and transported taxa. Sherrod (1999) stated that taphonomic processes that act on diatoms in salt marshes include transportation (e.g. Vos and De Wolf, 1993), breakage and dissolution (e.g. Denys, 1991/2; Ryves *et al.*, 2001). These processes can act alone or in combination altering the autochthonous diatom assemblages resulting in taxa being selectively removed due to breakage or dissolution or introduced to an assemblage due to tidal transportation.

Pollen assemblages are also subject to processes that can introduce bias into the eventual fossil assemblage through the selective transport of fossils, or by differential production or destruction, in which only the most robust specimens survive. The mechanism of pollen dispersal can also have implications for pollen taphonomy, wind pollinated (anemophilous) plants are generally more prolific pollen producers than insect pollinated (entomophilous) taxa resulting in entomophilous plant pollen being under-represented in comparison to anemophilous plant pollen in both modern and fossil samples. Wind dispersed pollen grains with adaptations such as a low specific gravity and air sacs are very buoyant in the air with the potential to disperse over long distances giving a misleading impression of vegetation cover. Chymura *et al.* (1995) determined that pollen deposition and re-suspension on a tidal flat followed a pattern predicted by Postma (1967) similar to the deposition of fine-grained clastic sediments. However, Chymura *et al.* (1995) suggest the salt marsh is a homogenous sink for pollen grains. The complex processes of pollen destruction, differential deposition and re-suspension on the tide may therefore have implications for the precision of sea-level reconstructions. Chymura *et al.* (1995) indicated that using the total pollen assemblage is the most unbiased method.

When the modern microfossils were counted no attempt was made to separate out the allochthonous and autochthnous diatoms or pollen (e.g. Sherrod, 1999) because this study assumes that a mixture of allochthonous and autochthonous diatom valves will also occur in the fossil sediment samples (e.g. Zong, 1997). Therefore, the total diatom and pollen assemblages have been used in this investigation as they are thought to most closely resemble the fossil assemblages.

3.7 STATISTICAL METHODS

Multivariate analysis techniques are used to simultaneously examine many environmental variables and is an invaluable tool when studying complex patterns and trends in ecological data; the results of which are normally presented in a simple graphic form, for example, a scatterplot or dendrogram, enabling the major patterns to be studied and interpreted easily.

The relationship between the diatom and pollen distributions and the modern environmental variables is explored using Detrended Canonical Correspondence Analysis (DCCA) and Canonical Correspondence Analysis (CCA) (ter Braak, 1986, 1987b).

The quantitative prediction of the reference water level from diatom, pollen and multi-proxy assemblages is a two-step procedure. Regression analysis establishes a model from a training set of modern surface data. Calibration of the fossil core/monolith samples is then used to infer past elevations of the salt-marsh surface from fossil data (Birks *et al.*, 1990). The set of mathematical equations by which this calibration is conducted forms a transfer function. The benefits of transfer functions are that they provide quantitative estimates that enable relative sea-level change to be reconstructed throughout the entire fossil sediment profile.

3.7.1 Detrended Canonical Correspondence Analysis

Detrended Canonical Correspondence Analysis (DCCA) is an ordination technique used to discover whether linear or unimodal statistical methods are appropriate for the available training set in relation to environmental variable(s) of interest. DCCA (ter Braak, 1986, 1987c) with *x* as the only environmental or external predictor variable and detrending by segments and non-linear rescaling provides an estimate (as the length of DCCA axis 1) of the gradient length in relation to *x* in Standard Deviation (SD) units. If the gradient length is short (<2 SD units), taxa are generally behaving monotonically along the gradient and linear regression and calibration are appropriate. If the gradient length is longer (>2 SD units), several taxa will have their optima located within the gradient and unimodal-based methods of regression and calibration are appropriate (Birks, 1995).

3.7.2 Canonical Correspondence Analysis

Canonical Correspondence Analysis (CCA) is calculated using CANOCO version 4.51 (ter Braak and Smilauer 1997-2003, see ter Braak, 1988, 1990). CCA (ter Braak, 1986) is a multivariate direct gradient analysis method derived from correspondence analysis but can also incorporate environmental data into the analysis. CCA is utilised to explore the relationship between modern pollen and diatoms and the environmental variables. CCA extracts synthetic environmental gradients from ecological data sets that can be used to illustrate and describe the different habitat preferences (niches) of taxa via an ordination diagram.

The results of the CCA are plotted as an ordination diagram using CanoDraw for Windows 4.1 (Smilauer, 1999-2003). The data can be displayed as taxa and environmental variables, or as samples and environmental variables, whereby the environmental vectors are overlaid on each graph. The environmental variables appear as arrows emanating from the centre of the graph indicating the direction of maximum change of that variable across the diagram (environmental gradient). For example, if an arrow for elevation points to the right of the diagram, elevation is increasing along an environmental gradient from left to right. The length of the arrow indicates the rate of change, a very long arrow indicates that elevation is strongly correlated with the ordination axis and therefore also with the species composition in the assemblages shown on the diagram, or with the adjacent taxa depending on whether it is a species or sample diagram. If the environmental variables show a strong relationship with the ordination axes (especially axis 1 and 2), they can account for the majority of variance in the species composition within the assemblages and can potentially be sufficient to predict variation in species composition (ter Braak, 1986).

The results are also presented as a correlation matrix (Table 4.2) for the environmental variables and a summary of the eigenvalues for the first four axes, which represents the variance explained by each axis. The "total inertia" in a data set is analogous to the variance. For unimodal methods the total inertia represents the variance or spread of species scores.

The percentage of explained variance is calculated as follows:

$$\frac{\text{Canonical eigenvalues}}{\text{Sum of all eigenvalues}} \quad \text{x} \quad \frac{100}{1} \quad = \quad \begin{array}{l}\text{Explained variance as a}\\ \text{result of environmental variables}\end{array}$$

3.7.3 Unimodal or linear regression and calibration methods?

The results of the DCCA determine whether unimodal or linear regression and calibration methods are appropriate. If the statistical analysis indicates that it is appropriate to assume a unimodal taxon-environment response model, regression methods such as Weighted Averaging (WA) regression and calibration with inverse and classical de-shrinking (e.g. Gasse *et al.*, 1995; Horton *et al.*, 1999; Zong & Horton 1999) and Weighted Averaging-Partial Least Squares (WA-PLS) (e.g. Sawai *et al.*, 2004; Hamilton, 2003; Woodroffe, 2006) can be used.

If the taxa show a linear distribution linear-based regression methods such as Partial Least Squares (PLS), Imbrie & Kipp Factor Analysis (IKFA) and Principal Components Analysis (PCA) can be used.

If the gradient length is between 2-3 standard deviation units the linear technique Partial Least Squares (PLS) will also be applied to ensure that the best model is used for these datasets that fall between linear and unimodal distributions. Birks (1998) suggests that in these cases WA-PLS usually outperforms the linear technique Partial Least Squares (PLS) because WA-PLS generally requires fewer components to create a minimal adequate model. In fact Birks (1995) suggests that WA-PLS is the most reliable and robust of all the transfer function models.

3.7.4 Transfer function (TF)

In this investigation the modern pollen, diatom and combined multi-proxy diatom and pollen data sets were used to develop transfer functions to enable the reconstruction of the magnitude of relative land and sea level changes. The primary aim of a transfer function is to express the value of the environmental data (e.g. elevation) or as a function of the biological data (the modern microfossil assemblages, so called proxy data). This function is termed the transfer function or biotic index (ter Braak, 1987a) and its construction is called "Calibration" by statisticians (ter Braak, 1987b; ter Braak & Prentice, 1988). It involves the use of linear regression to model the response of a biological taxon as a function of one or more environmental variables (Birks, 1995). As applied to this study, this usually involves a modern training set of taxa from many sites, studied as assemblages from the modern surface sediment under investigation, and an associated suite of modern environmental variables. Calibration is the opposite of regression, whereas regression models the response of the assemblage to an environmental variable, calibration estimates the value of the environmental variable, for example elevation, for the fossil assemblage by modelling the response of the same modern taxa today in relation to elevation. The relationship between the modern training set and elevation is modelled statistically and the resulting function is then used as a transfer function to transform the fossil data into quantitative estimates of elevation.

The performance of each transfer function will be evaluated by looking at the statistical parameters produced during regression. The choice of component depends upon the root-mean square of the error of prediction (RMSEP) and the squared correlation (r^2) of observed versus predicted values and the principle of parsimony, defined as choosing the lowest component that gives an acceptable model. The RMSEP is described as a measure of the predictive abilities of the training set and it can be used to assess the prediction errors. r^2 is indicative of the strength of the relationship between the observed and predicted values and this value allows comparison between transfer functions using different environmental variables. The RMSEP is the most robust value when considering the predictive error or predictive abilities of the training set as it incorporates a method of cross validation. The simplest and one of the most commonly used cross validation methods is jack-knifing or "leave-one-out" (ter Braak and Juggins, 1993). The results of this are expressed as the $\text{RMSEP}_{(\text{jack})}$, which is thought to be a more consistent measure of the predictive abilities of the transfer function. Another cross validation method called bootstrapping will be used in this research. Bootstrapping generates independent test sets from the original training set of sampling sites and generates sample specific errors and can be used to derive $\text{RMSEP}_{(\text{boot})}$ for individual fossil samples. This method is preferable as it generates sample specific errors.

3.7.5 Modern Analogues

It is very important to test the reliability of the transfer function to determine whether the resulting estimates of reference water level (RWL), are prone to errors due to no analogue and poor analogue situations. The statistical parameters produced by calibration and regression (e.g. RMSEP & r^2) provide information regarding the performance of the transfer function but do not provide any information on the reliability of the subsequent reconstructions. Modern analogue technique (MAT) offers a statistical method for assessing a good match between modern and fossil samples by producing a cut off point, beyond which samples are not considered a good match.

In its simplest form MAT was defined by Brew and Maddy (1995) as a technique to compare numerically, using an appropriate dissimilarity or similarity measure, the biological assemblage in a fossil sample with the biological assemblages in all available modern samples that have associated environmental data (i.e. the training set). MAT is a technique used to reconstruct a past environmental variable from modern microfossil assemblages. Having found a modern sample(s) that are similar to the fossil sample, the past environment for that sample is inferred to be the modern environment for the analogous modern samples(s). This procedure is then repeated for each of the fossil samples and a simultaneous reconstruction for several environmental variables is produced for the stratigraphical sequence on the basis of the modern training samples in the training set (e.g. Hutson, 1980; Prell, 1985; Morley 1989b; Anderson *et al.*, 1989 and Le, 1992). This method is therefore very useful in environmental reconstructions as it can be used to identify whether fossil samples have good modern analogues to highlight any inadequacies in the data due to differences in taxonomy, taphonomy, post depositional changes and anthropological effects (e.g. Edwards & Horton, 2000; Zong *et al.* 2003; Kucera *et al.* 2004).

Computer programmes such as C2 (version 1.4 beta, Juggins, 2003) have been used to run the modern analogue technique and many authors have used MAT successfully to identify fossil samples with poor modern analogues and to test the reliability of transfer function results in a variety of studies (e.g. Edwards and Horton, 2000; Gonzales-Donoso *et al.*, 2000; Muller *et al.*, 2003; Zong *et al.*, 2003; Edwards *et al.*, 2004; Kucera *et al.*, 2004; Hamilton *et al.*, 2005). However, recent studies (e.g. Woodroffe, 2006) have found the MAT problematic. Problems associated with the methodology (Birks, 1995) include difficulties if the modern training set is not of consistent taxonomy and quality, and the modern samples are not from the same type of sedimentary environment as the fossil datasets (Birks, 1994). Secondly, there are problems associated with how to measure the dissimilarity between modern and fossil assemblages. Squared chord distance and other coefficients such as squared chi-squared distance may be used for other problems and datasets to maximise the "signal to noise" ratio, however, the concept of similarity between assemblages is still complex. An additional problem is how to assess if the lowest dissimilarity found between a fossil sample and a modern sample represents a good match and analogue. It is misleading to determine that modern and fossil assemblages with low dissimilarity are necessarily good analogues (e.g. Huntley, 1990) because in any comparison, one of the samples has to have the lowest dissimilarity. All of the modern samples may be dissimilar to the fossil samples, but the computations will determine one sample the most dissimilar even if it is not statistically different from the other dissimilar samples. This can be overcome by taking the extreme 5% or 10% of the calculated dissimilarities between the modern samples as an approximate threshold value to indicate a "good analogue" (Anderson *et al.*, 1989; Bartlein & Whitlock, 1993). Alternatively, permutation tests (Manly, 1991) can be used to asses approximately the statistical significance of an observed dissimilarity value by permutating the fossil and modern assemblage many times, subject to certain constraints, and deriving an approximate empirical statistical distribution of the dissimilarity values to enable limits to be set for a "close" or "good" analogue with regard to the extreme 2.5% and 5% tails of the empirical distribution of dissimilarity coefficients.

Once the calibration process is completed for each transfer function model chosen values of RWL will be estimated for each of the fossil assemblages. To test the reliability of each of the RWL reconstructions the reliability of the reconstructions must still be assessed using methods other than MAT. The results can be compared with the sediment stratigraphy (lithology) and the microfossil assemblages to see how reliable the results are and to determine the precision of the reconstruction I can look at the size of the associated errors. For example, peat formation usually occurs at or above Mean High Water Spring (MHWS) tidal levels, so to determine how accurate the reconstructions are it is possible to compare the RWL for the point where peat formation commences with the MHWS tidal data at the location of the nearest tidal prediction. In addition, because the reconstructed RWL is more likely to be reliable if the fossil sample has close modern analogues in the training set simple mathematical methods can be employed. To identify fossil samples with poor analogues Birks (1998) suggests two simple independent measures of reconstruction reliability.

1. Percentage of the total fossil assemblage that consists of pollen or diatom taxa not represented in the modern training set.
2. Percentage of the total fossil assemblage that consists of taxa that have a low species abundance in the training set (e.g. <5% or <10%).

The first method will be used in this research as a simple measure of reconstruction reliability by calculating the percentages of fossil taxa that are present in the modern training set.

3.8 Summary

This chapter provides an outline of the main techniques used in this research to collect prepare and analyse the modern and fossil samples and the associated environmental data. This chapter then explains the statistical methods used to develop transfer functions (DCCA, CCA, transfer functions – regression and calibration and MAT). The following chapters will present the results of the transfer functions and the calibration of the fossil data to produce quantitative estimates of reference water level (RWL).

Chapter 4 Results: Development of a Transfer Function

4.1 INTRODUCTION

This chapter aims to describe the relationship between modern diatom and pollen assemblages from tidal flat to freshwater environments and a range of environmental variables. It will investigate the quantitative relationship between these assemblages and elevation in order to develop transfer function models for reconstructing past sea-level changes from fossil cores (Chapter 5). In order to investigate effects of spatial scale on transfer function applications, separate data sets from Kintail, Morar and Argyll give local, or site scale analyses, and combining the three datasets give regional scale analyses. This Chapter also contrasts diatom-based transfer functions with pollen-based transfer functions, and with combined (multi-proxy) diatom and pollen transfer functions.

This combination of three separate local scale analyses, one regional scale analysis and three different combinations of microfossils produces 12 separate permutations of modern datasets. In order to minimise repetition, section 4.2 and the accompanying figures and table describe in detail the procedures followed in determining the optimum transfer function model using the full diatom training set. Sections 4.3 – 4.5 onwards then summarise the results of the other permutations, referring only to key figures and tables.

The basic procedure followed is:

1. Detrended Canonical Correspondence Analysis (DCCA) is carried out to establish whether unimodal or linear regression models are applicable. Birks (1995) suggests that if the resultant gradient length is short (<2 SD units), taxa are generally behaving monotonically along the gradient and linear regression and calibration are appropriate. If the gradient length is longer (>2 SD units), several taxa will have their optima located within the gradient and unimodal-based methods of regression and calibration are appropriate.

2. Canonical Correspondence Analysis (CCA) is used to investigate the strength of relationship between elevation, other environmental variables and microfossil assemblages. In all cases elevation is shown as Standardised Water Level Index (SWLI) to allow for tidal range differences between sites.

3. Transfer Function model development, using different statistical measures (bootstrapped r^2, RMSE and RMSEP) along with scatter plots of observed against predicted elevation and scatter plots of residuals, to determine the number of components to consider. Criteria for the best model is to maximise r^2, minimise RMSE and RMSEP, minimise non-linearity in observed versus predicted, minimise trend in residuals, and minimise the number of components used. These may not all occur depending on the properties of the dataset, but each model will be considered in turn according to the statistical measures produced.

4.2 REGIONAL DIATOM TRAINING SET

116 modern diatom data from Kintail, Morar and Argyll form the regional training set (figure 4.1). The diatom samples have environmental data associated with them, all 116 of the samples have elevation (SWLI) data and 73 of the 116 samples also have associated salinity, LOI, pH and sediment grain size (% sand, % silt & % clay).

Figure 4.1 illustrates the dominant diatom species in the regional diatom training set. The dominant species change along the environmental gradient from the tidal flat at a low SWLI to the high marsh at a high SWLI (a SWLI value of 100 = MTL, a SWLI value of 200 = MHWS). A trend can be seen moving from the left of the diagram to the right with the highest percentage abundance of fully marine species (polyhalobous) e.g. *Cocconeis scutellum* and brackish species (mesohalobous) e.g. *Achnanthes delicatula* through oligohalobous-halophilous and oligohalobous-indifferent species e.g. *Navicula mutica* and *Hantzschia amphioxys* respectively. Finally, at the right of the diagram the diatom species are representative of freshwater environments dominated by halophobous species such as *Eunotia arcus*, *E. exigua* and *Pinnularia subcapitata*. This illustrates that the diatom assemblages are responsive to environmental change and the community structure of the assemblages are as a result of elevation (SWLI) and a variety of other environmental variables. This responsiveness indicates that the diatoms in the training set have the potential to be used to successfully develop transfer function models. Birks (1994) states that "one of the major requirements of any quantitative palaeo-environmental reconstruction is that the biological data, i.e. the microfossils have abundant identifiable fossils that are responsive and sensitive to the environmental variable of interest today at the spatial and temporal scales of study".

4.2.1 Regional Diatom Detrended Canonical Correspondence Analysis

As the length of axis 1 (Table 4.1) in standard deviation (SD) units is greater than two SD units for the full modern diatom training set unimodal methods of regression and calibration are appropriate.

4.2.2 Regional Diatom Canonical Correspondence Analysis

Canonical Correspondence Analysis (CCA) produces three pieces of information; a correlation matrix showing the relationship between the environmental variables (Table 4.2), Eigenvalues (Table 4.3) which allow the percentage of explained and unexplained variance to be calculated (Table 4.4) and indicate the relative importance of each of the axes in explaining the variance in the diatom assemblages, and ordination plots that illustrate the importance of each of the environmental variables.

The ordination plot (figure 4.2) illustrates the samples and their relationship to the environmental variables. In this ordination diagram, or bi-plot, the length of the arrow for each environmental variable approximates its relative importance in explaining the variance in the diatom data. The orientation of the arrows illustrates their approximate correlations to the ordination axes and the other environmental variables (e.g. Gasse *et al.*, 1995). The important factor to consider is the orientation and length of the elevation (SWLI) arrow (annotated SW), as this is the environmental variable that will be used in the transfer functions to reconstruct former sea-levels. Figure 4.2 illustrates that elevation, expressed as SWLI on the sample-environment bi-plot has the longest arrow, therefore elevation is the most important variable explaining the variance in the regional diatom training and LOI and pH are almost equally important, indicating that the primary environmental variable that will be reconstructed is SWLI. In addition to their proximity and orientation in figure 4.2, the correlation matrix (Table 4.2) also indicates that elevation (SWLI) is highly correlated with LOI (0.59) and negatively correlated to pH (-0.47). Salinity and the percentages of sand, silt and clay all have much shorter arrows and therefore are responsible for less of the variance within the diatom assemblages.

Figure 4.2 and table 4.3 show that axis one is correlated with elevation (SWLI), LOI, pH, salinity, silt, clay and sand. Axis one illustrates a major gradient from high marsh plotted on the left (high SWLI, LOI and % of silt and clay and low pH, % of sand and salinity) to tidal flat plotted on the right (low SWLI, LOI and % of silt, % of clay and high pH, salinity and % of sand).

Table 4.3 shows the CCA results as a summary of the eigenvalues showing the total variance (total inertia) in the diatom data (7.63). A simple calculation shows that the environmental variables investigated explain 26% of the total variance (Table 4.4). The remaining 74% represents inter-correlations between the variables and unexplained variance. The higher the percentage of variation that is explained the better the relationship between the modern diatoms and the environmental variables and the better they will be for use as a training set to reconstruct environmental change.

4.2.3 Regional Diatom Transfer Function (regression)

One of the basic requirements to adequately model the complex, non-linear, often unimodal relationships between modern taxa and their environment is that robust statistical methods for regression and calibration are used (Birks, 1994). It is therefore important to choose a suitable model determined by the underlying taxon-environment response assumed by the different methods (Birks, 1995). Non-linear unimodal-based methods include weighted averaging regression and calibration (WA) and weighted averaging partial least squares regression (WA-PLS).

Although for comparison both WA and WA-PLS regression will be carried out on the full diatom training set, WA-PLS is the preferred model (e.g. Sawai *et al.*, 2004; Hamilton, 2003; Woodroffe, 2006). ter Braak and Juggins (1993) identified that weighted averaging has three weaknesses. Firstly, ter Braak and Looman (1986) identified that WA is sensitive to the distribution of the sample sites within the training set along the environmental gradient of interest. Secondly, WA considers each environmental variable separately. Thirdly, WA disregards the residual correlations in the biological data, i.e. correlations that remain in the biological data after fitting the environmental variable and that are often caused by environmental variables that are not considered in WA. WA-PLS incorporates partial least squares regression into WA to overcome some of these weaknesses by taking into account residual correlations in the biological data to improve the estimations of the optima for the taxa (Birks, 1995). Birks (1995) states that "for data that span an environmental gradient of 2 or more SD units, WA-PLS is an appropriate and robust reconstruction procedure".

Table 4.5 shows the statistical parameters produced during the modelling process for all 116 samples from the regional diatom training set. To determine which model performs best it is important to understand what the results show. The standard error, or root mean square error (RMSE) is often quoted as a measure of the predictive capabilities of the training set as it assesses the prediction errors. The coefficient of determination (r^2) is a measure of the strength of the relationship between observed and inferred values and allows comparisons between transfer functions for different environmental variables (Gasse *et* al., 1995). As Birks (1994) suggested that "reliable and realistic statistical estimation of standard errors of prediction for the modern training set as a whole and for each reconstructed value is required" a method of cross validation is usually employed. In this investigation jack-knifing (leave-one-out) (ter Braak and Juggins, 1993) and bootstrapping (e.g. Efron, 1982; Efron and Gong, 1983) methods of cross validation have been used for comparison. This produces a measure of the predictive abilities of the training set called the root mean square error of prediction $RMSEP_{(jack)}$ or $RMSEP_{(boot)}$ after cross validation and $r^2_{(jack)}$ and $r^2_{(boot)}$ which are the coefficients of determination when a cross validation method has been used.

During transfer function model development the statistical measures (RMSE, $RMSEP_{(jack)}$, $RMSEP_{(boot)}$, r^2, $r^2_{(jack)}$ and $r^2_{(boot)}$) (table 4.5) produced along with scatter plots of observed against predicted elevation (SWLI) and scatter plots of residuals (Figure 4.3) can be used to determine the number of components to consider. Criteria for the best model is to maximise r^2, minimise RMSE and RMSEP, minimise non-linearity in observed versus predicted, minimise trend in residuals, and minimise the number of components used. As one of the basic requirements of any quantitative palaeo-environmental reconstruction is the production of sample-specific standard errors of prediction (Birks, 1994), bootstrapping is the chosen method of cross validation as it produces sample specific standard errors of prediction for both the individual fossil samples, as well as for all individual modern training samples.

Table 4.5 shows the resultant statistical parameters for the potential WA and WA-PLS models using jack-knifing and bootstrapping cross validation methods. The results indicate that WA-PLS performs better than WA giving higher r^2, $r^2_{(jack)}$ and $r^2_{(boot)}$ values and lower RMSE and $RMSEP_{(boot)}$ and $RMSEP_{(jack)}$ values. Model 1, weighted averaging partial least squares (WA-PLS) using component 3 is the chosen model as it has a low RMSE value and a high r^2 (0.94) the lowest $RMSEP_{(boot)}$ value (24.89) and the highest $r^2_{(boot)}$ value (0.83). The r^2 values obtained for model 3 (0.94) are comparable to, and improve upon the r^2 values obtained in other studies (Table 4.6). Campeau *et al.* (1999) suggest that an r^2 value > 0.9 indicates a good correlation. The full results of all the transfer function models are shown in appendix 1.

Figure 4.3 shows the regression results for the regional diatom training set for the first three components and the associated regression residuals. Figure

4.3 illustrates visually that component 3 produces a more linear relationship between the observed and predicted/estimated values of elevation (SWLI) and that the trend in the residuals has been reduced. The spread of regression residuals on the scatterplots (figure 4.3) indicate the distance from a line of perfect fit that the estimates of elevation (SWLI) occur. Sample points occurring above 0 indicate that those samples are over-estimating elevation (SWLI) and those occurring below 0 are under-estimating elevation (SWLI). The samples on or very near to 0 are performing well. Therefore, the nearer to zero the values are the better the model. Visual analysis of the trend in residuals suggests that the samples below an elevation of 100 SWLI are over-estimating SWLI and the samples from an elevation between 100 – 250 SWLI show a mixture of over and under-estimation when predicting elevation (SWLI) and show a tendency to under-estimate above 250 SWLI.

The regional training set WAPLS component 3 has a $RMSEP_{(boot)}$ value of 24.83 when the SWLI value of $RMSEP_{(boot)}$ is converted into m OD this gives a $RMSEP_{(boot)}$ value of 0.58 m at Nonach, 0.52 at Mointeach Mhor North and 0.36m at Barr-na-Criche. This equates to approximately one quarter of the altitude between MTL and MHWS. When this transfer function is applied to the fossil data there will also be errors associated with the goodness of fit between the modern and fossil diatom assemblages.

4.3 LOCAL DIATOM TRAINING SETS

The remaining local diatom training sets are from Kintail, Morar and Argyll. The Kintail modern diatom training set comprises 43 samples, 12 from Balmacara, 13 from Nonach and 8 from Eilean-nan-Gall. Only SWLI data is available for these samples. The Morar modern diatom training set comprises 22 samples from Saideal-nan-Ceapaich. 52 modern diatom samples, 37 from Loch Creran and 15 from Barr-na-Criche form the Argyll training set. Elevation (SWLI), pH, salinity, LOI, % sand, % silt and % clay data is available for both Morar and Argyll.

The three remaining local diatom training sets from Kintail, Morar and Argyll (Figures 4.4 – 4.6) all show a similar trend to the regional diatom training set.

The dominant species change along the environmental gradient from the tidal flat at a low elevation (SWLI) to the high marsh at a high elevation (SWLI). They all similarly show a trend moving from the left of the diagram to the right with the highest percentage abundance of fully marine species (polyhalobous) at the left of the diagram (e.g. *Cocconeis scutellum*) through to brackish species (mesohalobous) and oligohalobous-halophilous and oligohalobous-indifferent species and finally, at the right of the diagram the diatom species are representative of freshwater environments dominated by halophobous taxa. This illustrates that the diatom assemblages at each location are responsive to environmental change and the community structure of the assemblages are as a result of elevation (SWLI) and a variety of other environmental variables.

4.3.1 Local Diatom Detrended Canonical Correspondence Analysis

The length of axis 1 in standard deviation (SD) units is greater than two for the remaining local diatom training sets (Table 4.1) indication that unimodal-based methods of regression and calibration are appropriate.

4.3.2 Local Diatom Canonical Correspondence Analysis

The results of the CCA are shown in Tables 4.7 – 4.8 and Figure 4.7. As only elevation was measured at the sites in Kintail a correlation matrix and ordination plot have not been produced. The correlation matrices for Morar (Table 4.7a) and Argyll (Table 4.7b) show similar patterns of correlation. Elevation (SWLI) has a positive correlation with salinity, pH and the percentage of sand and has a negative correlation with LOI, the percentage of silt and the percentage of clay.

Table 4.8 a- c shows a summary of the eigenvalues for the CCA and table 4.4 lists the explained and unexplained variance in the datasets in comparison to the environmental variables. Elevation at Kintail explains 11% of the variance in the diatom data. The complete suite of variables explains 51 and 34% of the variance in the diatom data for Morar and Argyll respectively. This indicates that the Morar diatoms show a very strong relationship with the environmental variables. In fact both Morar and Argyll diatoms have a stronger relationship with the environmental variables that the regional training set.

The ordination diagrams for Morar (figure 4.7a) and Argyll (4.7b) indicate that at Morar the percentage of sand and SWLI have the longest arrows and explain much of the variance in the Morar training set. The Argyll ordination diagram illustrates that SWLI has the longest arrow and explains much of the variance in the training set.

4.3.3 Local Diatom Transfer Function (Regression)

Table 4.8 shows a summary of the transfer function performance statistics for each of the models chosen. All of the models give acceptable results, and comparison with table 4.6 indicates that the r^2 values are equal to and improve upon the r^2 values calculated in other studies. Interestingly, Morar, which had the strongest relationship to the environmental variables, has the highest r^2 value and is most precise as it has the lowest RMSE and RMSEP values.

Figures 4.8 – 4.10 illustrate the regression results for the Kintail, Morar and Argyll diatom training sets using the appropriate component on the left and the associated regression residuals are shown on the right. These figures all indicate a linear relationship between the observed and predicted/estimated values of elevation (SWLI). Although the trend in the residuals has been reduced there is still evidence of a trend. The spread of regression residuals on the scatterplots indicates the distance from a line of perfect fit that the estimates of elevation (SWLI) occur. All three diagrams show an over-estimation of SWLI at low elevations and an under-estimation of SWLI at higher elevations.

The local diatom training sets at Kintail, Morar and Argyll produce $\mathrm{RMSEP}_{(\mathrm{boot})}$ values of 27.79, 12.46 and 24.06 respectively. When applied to the fossil cores excluding additional errors due to goodness of fit the training sets would have error values of 0.64, 0.29 and 0.56 m at Nonach; 0.58, 0.26 and 0.51 m at Mointeach Mhor North and 0.41, 0.18 and 0.35 m at Barr-na-Criche. The

Morar training set is the most precise of the diatom training sets, including the regional training set.

4.4 POLLEN TRAINING SETS

The regional pollen training set comprises 82 samples from Kintail, Morar and Argyll. All 82 of the pollen samples have elevation (SWLI) data but the 25 samples from Kintail only have elevation (SWLI) data so 57 of the 82 samples also have associated salinity, LOI, pH and sediment grain size (% sand, % silt & % clay) data in addition to the elevation data. The Kintail pollen training set has 25 modern pollen samples, 4 from Balmacara, 16 from Nonach and 5 from Eilean-nan-Gall and only elevation (SWLI) data. The Morar training set comprises 15 samples from Saideal-nan-Ceapaich, and the Argyll pollen training set comprises 42 modern pollen samples, 27 from Loch Creran and 15 from Barr-na-Criche. Elevation (SWLI), pH, salinity, LOI, % sand, % silt and % clay data is available for the Morar and Argyll samples.

Figures 4.11 – 4.14 illustrate the dominant pollen types encountered in the various pollen training sets. All of the training sets display a change along an environmental gradient from the low marsh at low elevation (SWLI) to the high marsh at high elevation (SWLI). The samples taken from areas of low elevation (SWLI) tend to have higher abundances of salt marsh indicator species such as *Plantago maritima* and *Glaux maritima* and other organisms such as dinoflagellate cysts and foraminifera test linings and a high proportion of tree pollen. The mid-high marsh tends to have more cyperaceae, gramineae and herbaceous plants with fewer saltmarsh indicator species. The high marsh and supra tidal areas have a variety of species depending on the training set indicative of habitats such as calluna heath, alder carr and acidic bog. This indicates that the pollen data are also sensitive to environmental change and the community structure of the assemblages occur as a result of elevation (SWLI) and a variety of other environmental variables.

4.4.1 Pollen Detrended Canonical Correspondence Analysis

The length of axis 1 in standard deviation (SD) units is less than two for all of the pollen training sets with the exception of Argyll (Table 4.1), therefore linear-based methods of regression and calibration are appropriate for the regional, Kintail and Morar training sets.

4.4.2 Pollen Canonical Correspondence Analysis

As there is only elevation data for Kintail the regional training sets will comprise a sub-set of the samples from Morar and Argyll. Therefore for the CCA analysis the regional training set comprises 15 samples each from Saideal nan Ceapaich and Barr-na-Criche and 27 from Loch Creran.

The correlation matrices for the regional (Table 4.10a), Morar (Table 4.10b) and Argyll (Table 4.10c) training sets show similar patterns of correlation. Elevation (SWLI) has a positive correlation with LOI and the percentage of sand and a negative correlation with salinity, pH and percentage of silt and clay.

Table 4.11 a - d shows a summary of the eigenvalues for the CCA and table 4.4 lists the explained and unexplained variance in the datasets in comparison to the environmental variables. Elevation at Kintail explains 16% of the variance (Table 4.4) in the pollen data. The complete suite of variables explains 28, 53 and 37% of the variance in the pollen data for the regional, Morar and Argyll training sets respectively. This indicates that once again the microfossils from Morar and Argyll show a very strong relationship with the environmental variables.

Figures 4.15 a – c illustrate the results of the CCA as ordination diagrams for samples and environmental variables for the regional, Morar and Argyll pollen training sets. The SWLI arrow is longest in each diagram indicating that elevation (SWLI) is the variable that explains most of the variance in the pollen training sets. This indicates that the pollen training sets have potential to be utilised to reconstruct former sea-levels.

4.4.3 Pollen Transfer Function (Regression)

Whereas the diatom and multi-proxy training sets have an underlying taxon-environment response indicating that unimodal methods of regression and calibration are appropriate, the pollen training sets, with the exception of the Argyll, indicate that linear-based methods of regression and calibration are appropriate. Linear-based methods of regression that can be used include principal components regression (PCR), partial least squares regression (PLS) and Imbrie & Kipp Factor Analysis (IKFA). PCR has previously been applied to pollen data to reconstruct past climates (e.g. Norton *et.al.*, 1986) but PCR has a number of problems associated with it (Birks, 1995), the most important being that PCR does not have an associated cross-validation procedure (Stone & Brooks, 1990). In this investigation partial least squares (PLS) analysis will also be carried out as PLS usually requires fewer components and gives a lower prediction error than PCR and more importantly can be computed using a cross-validation procedure (Birks, 1995).

Table 4.12 shows a summary of the transfer function performance statistics for each of the models chosen. The Morar, Argyll and Kintail training sets give acceptable results, and comparison with table 4.6 indicates that the r^2 values are equal to and improve upon the r^2 values calculated in other studies. However, Morar, which had the strongest relationship to the environmental variables, has the highest r^2 value and the lowest RMSE and RMSEP values.

Figures 4.16 – 4.19 illustrate the regression results for the Regional, Kintail, Morar and Argyll pollen training sets using the appropriate component on the left and the associated regression residuals are shown on the right. Figures 4.16 and 4.17 indicate a poor linear relationship between the observed and predicted/estimated values of elevation for the regional and Kintail training sets. Figures 4.18 and 4.19 illustrate that there is a more linear relationship between the observed and predicted/estimated values of elevation (SWLI) for the Morar and Argyll training sets. Although the trend in the residuals has been reduced there is still evidence of a trend (4.16 – 4.19) The spread of regression residuals on the scatterplots indicate over-estimation of SWLI at low elevations and an under-estimation of SWLI at higher elevations similar to the trend illustrated by the diatom training sets.

The regional, Kintail, Morar and Argyll pollen training sets produce $RMSEP_{(boot)}$ values of 50.89, 57.61, 18.44 and 43.29 respectively. When applied to the fossil cores excluding additional errors due to goodness of fit the training sets would have error values of 1.18, 1.34, 0.43 and 1.00 m at Nonach; 1.07, 1.21, 0.39 and 0.91 m at Mointeach Mhor North and 0.75, 0.85, 0.27 and 0.64 m at Barr-na-Criche. The Morar training set is the most precise of the pollen training sets, but the pollen regression analysis produces much larger errors, some of the errors exceed 1.0 m.

4.5 MULTI-PROXY TRAINING SETS

75 modern multi-proxy samples from Kintail, Morar and Argyll form the regional multi-proxy training set. All 75 of the diatom and pollen samples have elevation (SWLI) data and 52 of the 75 samples also have associated salinity, LOI, pH and sediment grain size (% sand, % silt & % clay) data. The Kintail multi-proxy training set comprises 23 samples, 4 from Balmacara, 16 from Nonach and 3 from Eilean-nan-Gall. Only elevation (SWLI) data is available for these samples. 15 modern multi-proxy samples from Saideal-nan-Ceapaich form the Morar training set and 37 modern diatom and pollen samples, 27 from Loch Creran and 10 from Barr-na-Criche form the Argyll multi-proxy training set. Elevation (SWLI), pH, salinity, LOI, % sand, % silt and % clay data is available for both Morar and Argyll.

As one would expect the regional and local multi-proxy diatom and pollen training sets (figures 4.20 – 4.23) are also sensitive to environmental change and show similar trends to the single microfossil training sets along the environmental gradient from low elevation (SWLI) to higher elevation (SWLI).

4.5.1 Multi-proxy Detrended Canonical Correspondence Analysis

The length of axis 1 in standard deviation (SD) units is greater than two for the multi-proxy training sets (Table 4.1), therefore unimodal-based methods of regression and calibration are appropriate.

4.5.2 Multi-proxy Canonical Correspondence Analysis

Once again omitting Kintail, the regional multi-proxy training set comprises 15 samples from Saideal nan Ceapaich, 11 from Barr-na-Criche and 27 from Loch Creran. The correlation matrices for the regional (Table 4.13a) Morar (Table 4.13b) and Argyll (Table 4.13c) training sets show similar patterns of correlation. Elevation (SWLI) has a positive correlation with LOI and the percentage of sand and a negative correlation with salinity, pH, percentage of silt and clay as does the pollen training sets. With the exception of the Morar multi-proxy training set which shows that elevation (SWLI) has a negative correlation to LOI and has a very high positive correlation with the percentage of sand.

Table 4.14 a - d shows a summary of the eigenvalues for the CCA and table 4.4 lists the explained and unexplained variance in the datasets in comparison to the environmental variables. Elevation at Kintail explains 18% of the variance (Table 4.4) in the multi-proxy data. The complete suite of variables explains 28, 43 and 38% of the variance in the multi-proxy data for the regional, Morar and Argyll training sets respectively, figures comparable to the diatom and pollen data. Once again the microfossils from Morar and Argyll show a very strong relationship with the environmental variables.

Figures 4.24 a – c illustrate the results of the CCA as ordination diagrams for samples and environmental variables for the regional, Morar and Argyll multi-proxy training sets. The SWLI arrow is longest in each diagram indicating that elevation (SWLI) is the variable that explains most of the variance in the multi-proxy training sets. This indicates that the multi-proxy training sets have potential to be utilised to reconstruct former sea-levels.

4.5.3 Multi-proxy Transfer Function (Regression)

Where the multi-proxy training sets have an axis length (Table 4.1) in standard deviation (SD) units between 2-3 the linear technique Partial Least Squares (PLS) will also be applied to ensure that the best model is used for these datasets that fall between linear and unimodal distributions. However, Birks (1998) suggests that in these cases WA-PLS usually outperforms the linear technique partial least squares (PLS) because WA-PLS generally requires fewer components to create a minimal adequate model.

Table 4.15 shows a summary of the transfer function performance statistics for each of the models chosen. All of the multi-proxy training sets give excellent results, and comparison with table 4.6 indicates that the r^2 values improve upon the r^2 values calculated in other studies. Morar, which had the strongest relationship to the environmental variables still has the highest r^2 value and the lowest RMSE and RMSEP values. The multi-proxy regression results indicate that multi-proxy training sets will provide the most precise estimates. The standard error, or root mean square error (RMSE) is often quoted as a measure of the predictive capabilities of the training set as it assesses the prediction errors, and as the RMSE values are the lowest this should indicate that the reconstruction using multi-proxy training sets will be most precise. The coefficient of determination (r^2) is a measure of the strength of the relationship between observed and inferred values and allows comparisons between transfer functions for different environmental variables (Gasse, *et al.*, 1995). The Morar training set, which shows a strong relationship with the environmental variables in the CCA produces the highest r^2 values and the lowest RMSE and RMSEP values.

Figures 4.25 – 4.28 illustrate the regression results for the Regional, Kintail, Morar and Argyll multi-proxy training sets using the appropriate component on the left and the associated regression residuals are shown on the right. Figures 4.25 – 4.28 indicate a linear relationship between the observed and predicted/estimated values of elevation (SWLI) for the multi-proxy training sets. Although it is evident that below a SWLI value of 100 there are no samples available that contain both diatoms and pollen available for the analysis.

Although the trend in the residuals has been reduced there is still evidence of a trend (figures 4.25 – 4.28). The spread of regression residuals on the scatterplots indicate over-estimation of SWLI at lower elevations and an under-estimation of SWLI at higher elevations similar to the trend previously illustrated by both the diatom and pollen training sets.

To ensure that the results are directly comparable and are not just an artefact of sample size the transfer functions were computed again to compare the regional multi-proxy training set to regional training sets comprising the diatom and pollen samples from the multi-proxy training set so that exactly the same samples, and same number of samples were used (Table 4.16). The summary of the results (table 4.17) indicates that the multi-proxy training set once again performs best, followed closely by the diatom training set. The pollen training set once again has the poorest performance.

The regional, Kintail, Morar and Argyll multi-proxy training sets produce $\mathrm{RMSEP}_{(\mathrm{boot})}$ values of 17.90, 26.40, 11.65 and 15.93 respectively. When applied to the fossil cores excluding additional errors due to goodness of fit the training sets would have error values of 0.42, 0.61, 0.27 and 0.37 m at Nonach; 0.38, 0.55, 0.24 and 0.33 m at Mointeach Mhor North and 0.26, 0.39, 0.17 and 0.23 m at Barr-na-Criche. Once again the Morar training set is the most precise of the training sets, and the multi-proxy regression analysis produces the smallest RMSEP values, indicating that multi-proxy training sets are most precise.

When the diatom and pollen transfer functions are repeated using only the samples in the multi-proxy training set to allow a direct comparison the result is quite surprising. Even though the training sets now contain less samples, for example, the regional diatom training set consisted of 116 samples, 75 of which are included in the multi-proxy training set, the transfer function results suggest these training sets are more precise (see Tables 6.1 and 6.2 for results) than the original training sets containing all available samples.

4.6 Summary

Transfer function models have been developed in this chapter for the diatom, pollen and multi-proxy training sets. In Chapter 5 the transfer function models that demonstrated the best performance will be applied to fossil data from Nonach, Mointeach Mhor North and Barr-na-Criche, in the process called calibration (see page 40) to reconstruct RWL for each fossil core or monolith sample.

Chapter 5 Results – Reconstruction of former sea levels

5.1 INTRODUCTION

In Chapter 4, twelve transfer functions were developed comprising a regional training set and three local training sets to reconstruct the fossil reference water levels using modern diatom, pollen and diatom and pollen (multi-proxy) assemblages. In this chapter these transfer functions provide local and regional reconstructions of relative sea-level from Nonach, Mointeach Mhor North and Barr-na-Criche. These allow comparisons between the different microfossil reconstructions and those arising from regional versus site-specific transfer function models.

This chapter comprises.

1. A reconstruction of former sea-levels at Nonach using regional diatom, pollen and multi-proxy training sets and three local training sets from Kintail, Morar and Argyll.
2. A reconstruction of former sea-levels at Mointeach Mhor North using regional diatom, pollen and multi-proxy training sets and three local training sets from Kintail, Morar and Argyll.
3. A reconstruction of former sea-levels at Barr-na-Criche using a regional pollen training set and three local pollen training sets from Kintail, Morar and Argyll. Diatoms were not preserved in this fossil core therefore reference water level reconstructions using diatom or multi-proxy training sets were not possible.

Each reconstruction in this section produces figures showing the various microfossils recorded in each of the fossil cores/monoliths. The chosen transfer function model that demonstrated the best performance in Chapter 4 was applied to this microfossil data, a process called calibration (see section 3.7.4, page 40), the results of which are shown as a diagram of the reconstructed fossil reference water level (m OD). In Chapter 4 to ensure that the results of the transfer functions were directly comparable and not just an artefact of sample size the transfer functions were ran again using only the diatom and only the pollen data within the multi-proxy training set so that the same samples and same number of samples could be compared. This has also been employed in this chapter and for the diatom and pollen only reconstructions an additional RWL reconstruction has been produced using just the diatom data and just the pollen data within the multi-proxy training set to ensure the results can be directly compared with the multi-proxy results. To test the reliability each of the RWL reconstructions was assessed by comparing the results with the sediment stratigraphy (lithology), the microfossil assemblages and the size of the associated standard errors. For example, peat formation usually occurs at or above Mean High Water Spring (MHWS) tidal levels, so to determine how accurate the reconstructions are it is possible to compare the RWL at the point where peat formation commences with the MHWS tidal data at the nearest tidal prediction.

To allow comparison of the regional and local reference water level reconstructions for each core/monolith an X Y plot is produced for each of the regional reconstruction versus each of the local reconstructions, theoretically if the reconstructions are giving similar results the relationship between the regional and local reconstruction will be linear, therefore deviations from a diagonal line indicate where the reconstructions have differing estimates of reference water levels.

To compare the reliability of the reconstruction the percentage of microfossils in the modern training sets that are present in the fossil cores are presented in table 5.1. The results for the additional pollen and diatom reconstructions from the multi-proxy training sets are listed in Table 5.2.

The fossil cores are presented with the most northern fossil core at Nonach in Kintail first, then monolith sample MMN01 in Morar and finally, the most southerly fossil core at Barr-na-Criche in Knapdale, Argyll. The locations of the fossil cores are shown in Chapter 2.

5.2 NONACH

Fossil core NN04 originates from Nonach in Kintail, one of the sites where samples were collected for the modern training sets. Calibration of core NN04 produces three sets of results, one each for the diatom, pollen and multi-proxy reconstructions. Figures 5.1 – 5.3 show fossil core NN04 with a simplified lithology for ease of reproduction to the left, a summary of diatom, pollen and multi-proxy species exceeding 2% of the total and reference water level reconstructions for the regional and three local training sets on the right. This section reveals a basal organic sand grading upwards into an organic silt-sand and eventually into a peat at 45 cm. Microfossil and lithological analyses indicate sedimentation under the control of relative sea level change. The diatom data (figure 5.1) indicates that the organic sand and organic silt sand are marine in origin and are dominated by the mesohalobous species *Diploneis interrupta* and fully marine (polyhalobous) diatom species. The peat layer still has polyhalobous and mesohalobous diatom species but up the core oligohalobous-halophilous (fresh-brackish) diatom species such as *Navicula pusilla* and *Pinnularia borealis* become more abundant suggesting a change from tidal flat, then low marsh to a tidal marsh community, with the exception of a peak of the epiphytic marine diatom *Cocconeis scutellum* at 40 cm, commonly found attached to marine algae washed up at the strand line at MHWS.

The pollen data (figure 5.2) indicates the organic silt sand is from a low marsh environment with pollen from salt-marsh indicator species such as aster type, *Glaux maritima*, *Armeria maritima* and *Plantago maritima* indicative of a tidal marsh community. This then grades into a fresh alder carr community with abundant alder (*Alnus*) and Gramineae and a decrease in salt-marsh indicator species. The multi-proxy" data (figure 5.3) indicate that the organic silt sand is dominated by the mesohalobous (marine-brackish) diatom species *Diploneis interrupta* and *Navicula peregrina* and Myrica-type, *Plantago maritima* and Gramineae pollen, representative of a tidal marsh environment. The peat layer shows an increase in oligohalobous-halophilous (fresh-brackish) diatom species and a decrease in *Diploneis interrupta* and an increase in pollen indicative of an alder carr habitat (*Alnus*).

5.2.1 Nonach diatom reconstructions

Figure 5.1 illustrates that the diatom reference water level (RWL) reconstructions for the regional and local diatom training sets all show a broadly similar trend with the exception of Morar. The stratigraphic and biological data suggest very little change then a fall in relative sea-level to present. The bio-stratigraphy suggests that the sediment in the organic sand at the base of the core was formed at a lower relative m OD with an increase in elevation in the organic silt-sand and an elevation above MHWS for the peat layer. However, the regional, Kintail and Morar reconstructions show a slight increase in the elevation of the RWL between 56 - 50 cm, then a slight decrease between 50 – 46 cm, an increase between 46 – 42 cm and finally a decrease in RWL between 42 – 40 cm. At 45 cm peat formation commences, it is expected that this will occur at approximately MHWS. The nearest tidal prediction to Nonach is at Dornie Bridge, where MHWS is 2.62 m OD. The precision of reconstructions can be evaluated by comparing the reconstructed reference water level (m OD) at 45 cm with MHWS at the nearest tidal prediction. The regional, Kintail, Morar and Argyll RWL reconstructions calculate the RWL at 3.02, 2.65, 3.07 and 3.14 m OD respectively, with sample specific errors of 0.37, 0.56, 0.35 and 0.37 m OD. Therefore, at 2.65 m OD, the Kintail training set RWL reconstruction is most accurate at this depth, only 0.03m greater than the MHWS at Dornie Bridge, whereas the remaining training sets all calculate RWL in excess of 3.0 m OD, but the Kintail training set has the largest sample specific errors of all the training sets so is therefore the least precise. At 40 cm, the high proportion of *Cocconeis scutellum* has an obvious effect on the reconstruction, as the estimated RWL is much lower than expected due to the high percentage of the marine species *Cocconeis scutellum.* The dominance of the intertidal species *Diploneis interrupta* may have influenced the RWL reconstruction resulting in very little change in the estimates of RWL.

The RWL reconstruction for the diatom data from the multi-proxy training set is displayed on the far right of figure 5.1. The results are very similar to the training set that contains all of the available diatom data except that at 40 cm the modern training set does not contain modern diatom samples from an environment on the tidal flat dominated by *Cocconeis scutellum*, and as a result does not estimate the RWL at such a low elevation. In general although the trend is similar the RWL for the regional diatom training set is continuously estimated approximately 0.6 m below the complete diatom training set. The Argyll and Morar datasets estimate the RWL below the regional training set and Kintail is very similar to the regional dataset, estimating only slightly higher. The Kintail training set still estimates the RWL where peat formation commences at 45 cm at 2.53 m OD, 0.09 m below MHWS at Dornie Bridge (2.62 m OD).

XY plots comparing the regional reconstruction with the local reconstructions for the diatom dataset (figure 5.4) illustrates the differences between the estimates of reference water level. Comparison of the diatom datasets indicates that the sample dominated by *Cocconeis scutellum* results in a lower estimation of RWL than the other samples and that the regional dataset and the Argyll dataset produce the most comparable estimates.

Tables 5.1 and 5.2 list the percentages of microfossils encountered in the fossil data that are also present in the modern training set. The regional diatom training set has the highest percentage of modern analogues with 89.2 % of the fossil diatoms also present in the modern training set. The local training sets from Kintail, Morar and Argyll have slightly fewer analogues, but the Kintail training set containing samples from the local area where core NN04 was taken has 83.1 % modern analogues. Table 5.2 shows the results for the diatom samples within the multi-proxy training set. These training sets have slightly lower percentages of modern analogues most probably due to the smaller size of the training sets but similarly the regional and Kintail training sets have a high percentage of modern analogues.

5.2.2 Nonach pollen reconstructions

The pollen RWL reconstructions (figure 5.2) show a different trend to the diatom data. The pollen RWL reconstruction indicates that at the base of the organic silt-sand the assemblages were formed at between 2.0 – 6.0 m with a slight decrease in RWL to 49 cm where the assemblages formed at a lower elevation and a fluctuating increase in RWL, or decrease in RSL to present. Morar and Argyll consistently calculate the RWL at a lower elevation than the regional training set and the Kintail training set estimates the RWL lower than the regional dataset between 54 – 46 cm and at higher elevations between 45 – 40 cm. At 45 cm, where peat formation commences, the regional, Kintail, Morar and Argyll datasets calculate the RWL at 3.91, 3.95, 2.72 and 3.15 m OD respectively with sample specific errors of 0.77, 1.11, 0.34 and 0.57 m OD. At this depth the RWL reconstruction using the Morar dataset is the most accurate, being 0.1 m OD above the MHWS at Dornie Bridge, and has the smallest sample error.

The pollen RWL reconstruction using only the pollen samples within the multi-proxy training set is illustrated at the far right of figure 5.2. There is a broadly similar trend with the lowest RWL estimates within the silt-sand and a gradual increase in RWL to present. However, between 54 and 49 cm the regional training set estimates the RWL below the training set containing all of the available samples. The Argyll training set consistently estimates RWL higher than the other datasets. Morar mostly estimates RWL above the regional training set; whereas the Kintail dataset mostly estimates RWL lower than the regional training set. Similarly Morar is still the most accurate reconstruction estimating the RWL at 2.69 m OD at 45 cm; 0.07m above MHWS at Dornie Bridge, and the estimate is most precise with a standard error of 0.21 m.

XY plots comparing the regional pollen RWL reconstruction with the local reconstructions (figure 5.5) illustrate the differences between the RWL estimates. Comparison of the pollen datasets indicates that once again the Argyll dataset and regional dataset provide the most comparable estimates of RWL although the regional reconstruction has consistently higher estimates of RWL compared to Argyll.

Tables 5.1 shows that the regional pollen training set has the most modern analogues with 87.9 %. On this occasion, of the local training sets, the Argyll pollen training set has the highest percentage of modern analogues (81.9 %). Table 5.2 showing the results for the pollen assemblages within the multi-proxy training set has slightly lower percentages of modern analogues due to the smaller size of the training sets and the Argyll pollen training set has a higher percentage of modern analogues than the regional training set.

5.2.3 Nonach multi-proxy reconstructions

The multi-proxy diatom and pollen RWL reconstructions (figure 5.3) show a trend in RWL that is more comparable to the stratigraphic and microfossil evidence. The regional dataset calculates the formation of the organic silt sand between 50 – 54 cm at 2.29 – 2.38 m OD, with a small decrease in RWL to 2.15 m OD (i.e. a small increase in RSL), then an increase in RWL, or fall in RSL to present to a RWL of 2.90 m OD at 40 cm. The Kintail and Morar RWL reconstructions follow a broadly similar trend, although on almost all occasions under estimate the RWL in comparison to the regional dataset, especially between 46 – 40 cm. The Argyll training set is much more erratic, being very similar to the regional dataset at 54, 51 and 50 cm, under estimating at 52, 46 - 42 cm and over-estimating at 40cm. At 45 cm where peat formation commences the RWL reconstructions for the regional, Kintail, Morar and Argyll datasets give values of 2.54, 2.44, 2.36 and 2.33 m OD respectively and errors of 0.22, 0.37, 0.25 and 0.19 m OD. Comparison with MHWS at Dornie Bridge (2.62 m OD) indicates that the regional dataset is most precise estimating the RWL at 0.08 m below MHWS.

XY plots comparing the regional multi-proxy reconstruction with the local reconstructions (figure 5.6) show the differences in the RWL estimates. The multi-proxy comparisons indicate that the regional and Kintail datasets produce the most similar estimates whereas the pollen and diatom comparisons show that the Regional and Argyll datasets provided the most similar estimates of RWL.

Tables 5.1 shows that the regional multi-proxy training set has the most modern analogues, 92.3 % and once again the Argyll pollen training set (81.3 %) is the local training set with the most modern analogues.

5.2.4 Nonach Summary

The diatom reconstruction at Nonach shows a gradual decrease in RWL to present as expected, with the exception of the assemblage at 40 cm. The local training set from Kintail, reconstructs the transition to a peat forming community most accurately at 2.65, 0.03 m above MHWS, however the Kintail training set is least precise with sample specific errors of 0.56 m. The Kintail diatom dataset containing only the diatom samples from the multi-proxy training set also reconstructs the transition to peat most accurately at 2.53 m OD, 0.09 m below MHWS at Dornie Bridge, but with a standard error of 0.40 m is the least precise, although it has smaller errors than the complete diatom training set.

The pollen reconstruction does not show an expected trend, since the minerogenic unit was formed at a higher elevation than the peat. In this instance the most local pollen training set is not the most accurate. The pollen training set from Morar including all available samples estimates peat formation at 2.72 m OD, 0.1 m above MHWS at Dornie Bridge and has a standard error of 0.34 m. The Morar training set that only includes the multi proxy samples also reconstructs the transition to a peat-forming environment most accurately at 2.69 m and with standard errors of 0.21m is most precise. In this instance the reconstruction using the pollen from the multi-proxy dataset is the most accurate and more precise, but does not give the expected results.

The multi-proxy reconstruction produces a reconstruction similar to what one would expect considering the stratigraphic and microfossil evidence. The multi-proxy reconstruction results indicate that the regional multi-proxy training set is the most accurate estimating the transition to a peat-forming community at 2.54 m OD 0.08 m below MHWS at Dornie Bridge. With a standard error of 0.22 the regional training set is not the most precise, for Argyll is with a standard error of 0.19 m.

The regional training sets contain the most modern analogues. The regional multi-proxy reconstruction has the greatest percentage of modern analogues with 92.3 % of microfossils in fossil core NN04 also present in the modern regional training set. The regional diatom training set has 89.2 % modern analogues and the regional pollen training set 87.9 %. The local diatom and multi-proxy training sets have 83.1 and 79.1 % modern analogues, whereas the pollen training set from Argyll provides good local modern analogues (81.8 %). The original training sets have more modern analogues than the lone pollen and diatom training sets from the multi-proxy dataset. The pollen from the multi-proxy dataset shows that Argyll has the most modern analogues.

5.3 MOINTEACH MHOR NORTH

Unlike Nonach to the north that only shows a regressive sequence, Mointeach Mhor North demonstrates a more complex transgressive sequence followed by a regressive sequence. Figures 5.7 – 5.9 show monolith MMN01AB at Mointeach Mhor North. This section reveals a basal peat grading upwards into a more minerogenic unit of organic silt-clay then organic silt-clay with sand then a peat with silt and clay and finally an upper herbaceous peat. When considering the stratigraphical and microfossil evidence the reference water level reconstruction should have the freshwater assemblages in the basal peat at a high elevation (reference water level m OD) at or above MHWS, then a decrease in RWL in the minerogenic organic silt-clay and organic silt-clay with sand indicative of the intertidal area, then an increase in RWL as RSL falls up the monolith to present until it reverts to a freshwater peat at 10 cm. Microfossil evidence corroborates the stratigraphic data. At 50cm the diatom data (figure 5.7) suggests that minerogenic sedimentation commences under intertidal conditions characterised by diatom assemblages dominated by the mesohalobous species *Diploneis interrupta* and the polyhalobous (fully marine) *Paralia sulcata*, found in both the plankton and benthos of coastal environments (e.g. McQuoid & Nordberg, 2003) and *Diploneis smithii*. The polyhalobous species *Rhabdonema minutum*, a marine intertidal diatom, is most abundant at 36 cm, indicating the peak of marine influence is within the organic silt-clay with sand. In the peat with silt and clay, moving up the core polyhalobous species e.g. *Diploneis smithii* begin to decrease and mesohalobous species e.g. *Caloneis westii* become more abundant. Changes in the pollen (figure 5.9) from the basal peat to the overlying minerogenic unit suggest an abrupt change from an acidic bog dominated by *sphagnum* and *calluna* to saltmarsh, indicating a rise in RSL. Shennan *et al.* (2005) attribute this transition to the breakdown of the dune system after being breached by the sea causing this rapid change in sedimentary environment and water salinity. Then after a peak of marine influence within the minerogenic unit RSL falls moving up the monolith and eventually the saltmarsh pollen decrease and at 10 cm a freshwater environment dominated by pollen indicative of alder carr (*Alnus*) dominates in the upper freshwater peat. The multi-proxy diatom and pollen data provides similar evidence. The organic silt-clay above the basal peat is dominated by polyhalobous and mesohalobous diatom taxa and pollen indicative of a marine environment, such as, Gramineae and *Armeria maritima,* then moving up the monolith *Diploneis interrrupta* decreases in abundance, *Rhabdonema minutum* increases in abundance, reaches a peak and decreases in abundance and pollen indicative of a saltmarsh environment begin to become more abundant, e.g. *Myrica*, and *Plantago coronopus.*

5.3.1 Mointeach Mhor North diatom reconstructions

The diatom RWL reconstructions (figure 5.7) do show a trend similar to that expected according to the stratigraphical and microfossil data, although there is an unexpected small increase in RWL in the organic silt-clay unit in the regional, Kintail and Morar dataset reconstructions before they fall to a minimum at 37 cm. These three training sets then all show a broadly similar trend of increasing RWL (falling RSL) between 37 – 20 cm, although Kintail has lower estimates for most of the reconstruction, and Morar is quite similar to the regional dataset reconstruction. Alternatively the Argyll training set, although in a similar range of RWL as the regional and Morar reconstructions has a more fluctuating pattern, where the other reconstructions show an increase in RWL in the lower minerogenic unit, the Argyll reconstruction has a small increase followed by a decrease in RWL and at 37 cm where the other three datasets estimate a fall in RWL, Argyll records an increase before showing a slightly increasing RWL trend to 20cm. The nearest tidal prediction to Mointech Mhor North is to the north at Mallaig, where MHWS is recorded at 3.38 m OD. Peat formation ends at 50cm in the basal peat and commences again at 33 cm. Comparison of the reconstruction values at these points to evaluate the accuracy of the reconstruction reveals that at 32 cm the regional, Kintail, Morar and Argyll reconstruction estimate a RWL of 2.46, 1.95, 2.51 and 2.32 m OD respectively, with sample errors of 0.32, 0.53, 0.19 and 0.33 m OD. The regional and Argyll datasets are most accurate at this depth, the regional reconstruction estimates 2.46 m OD, 0.08 m OD above MHWS and the Argyll dataset estimates the assemblage to have been accumulated at 2.32 m OD, 0.06 m OD below MHWS at Mallaig. At 50 cm the regional, Kintail, Morar and Argyll training sets estimate RWL at 2.52, 2.42, 2.58 and 2.20 m OD respectively; the Kintail dataset is most accurate at 2.42 m OD, 0.04 m above MHWS at Mallaig but with a sample specific standard error of 0.60 m is the least precise. At 32 and 50 cm the local training set from Saideal nan Ceapaich in Morar although not providing the most accurate reconstruction is most precise and has the smallest associated standard errors of 0.19 and 0.25 m respectively.

The RWL reconstruction containing just the diatom samples within the multi-proxy training set is shown on the far right of figure 5.7 to allow a direct comparison of the diatom reconstruction with the multi-proxy reconstruction (figure 5.9). Both RWL reconstructions are broadly similar, both showing a peak of marine influence within the organic silt-clay with sand. The original regional training set utilising all of the available samples has a broader range of estimated RWL, and the Morar and Argyll reconstructions for the diatoms samples within the multi-proxy training set are estimating RWL slightly lower than the regional training set, whilst the Kintail reconstruction is estimating RWL higher. Comparison of the performance of the reconstruction where peat formation commences at 32 cm indicates that the regional reconstruction estimating RWL at 2.18 m OD, with a standard error of 0.23 m OD is the most accurate at 0.2 m below MHWS at Mallaig. Whereas in the peat at 50 cm the Kintail RWL reconstruction is most accurate estimating RWL at 2.23 m OD, but with a standard error of 0.38 m is the least precise. The Morar training set reconstructions at 32 and 50 cm have standard errors of 0.13 and 0.14 m respectively are once again most precise.

XY plots comparing the regional diatom reconstruction with the local reconstructions (figure 5.10) show the differences in the RWL estimates. The comparisons indicate that the regional and Morar datasets produce the most comparable estimates of RWL. The Kintail reconstruction in particular consistently underestimates RWL.

Tables 5.1 shows that the regional diatom training set has the most modern analogues with 73.1 % and the local modern training sets have a smaller percentage of modern analogues, between 53.8 – 57.7 %. Table 5.2 showing the results for the diatom assemblages from the multi-proxy training set have slightly lower percentages of modern analogues.

5.3.2 Mointeach Mhor North pollen reconstructions

The pollen RWL reconstructions (figure 5.8) do not show a trend synchronous with the microfossil and stratigraphic data and the different dataset reconstructions are clearly affected by the length of the environmental gradient over which the modern samples were taken. Argyll, inclusive of the final modern microfossil sample at Barr-na-Criche taken at 5.73 m OD has higher estimations than the other reconstruction for most of the core. This in turn influences the regional dataset which estimates much higher reference water levels than the Kintail and Morar reconstructions. The modern pollen sample with the highest elevation at Morar within the TF model is at 2.30 m OD, therefore limiting the altitudinal range of the reconstruction. Within the Kintail TF the modern pollen sample with the highest elevation is at 6.02 m OD, although the Kintail reconstruction consistently estimates the RWL lower than the regional dataset. At 32cm the regional, Kintail, Morar and Argyll datasets estimate RWL at 3.55, 2.10, 1.89 and 4.55 m OD respectively, with sample errors of 0.74, 0.74, 0.24 and 0.82 m the errors for the regional are joint second largest, whereas the reconstruction at Morar has the smallest sample errors making it most precise. At 50 cm the regional, Kintail, Morar and Argyll datasets estimate RWL at 3.96, 2.92, 2.75 and 2.57 m OD respectively, with sample errors of 0.72, 0.87, 0.38 and 0.82 m OD. At 32 cm Kintail is most accurate at 2.10 m OD, 0.28 m below MHWS at Mallaig. At 50 cm the Argyll reconstruction is most accurate at 2.57 m OD, 0.19 m OD below

MHWS at Mallaig but the local training set from Morar, with a SE of 0.38 m provides the most precise reconstruction.

The pollen dataset containing only the samples within the multi-proxy training set, at the far right of figure 5.8, also display a similar trend to the dataset with all available samples, although the estimates of RWL in the minerogenic units are surprisingly more pronounced and still the opposite of what one would expect. The regional reconstruction estimates RWL lower than the training set containing all available samples. This could, for example, be because some of the samples at the landward end of the transect taken above 5.0 m OD are not included within the dataset. In turn this influences the regional training set and lowers the RWL estimation so it is more similar to those at Morar and Kintail. This indicates that the length of the sample transect, or more precisely the range over which the modern samples are taken can have a substantial impact on the reconstruction estimates of RWL. To assess how accurate the reconstruction is, the estimates of RWL at 32 and 50 cm are once again compared with the MHWS of 2.38 m OD at the nearest tidal prediction at Mallaig. At 32 cm with an estimate of 2.26 m OD Kintail is the most accurate estimate only 0.12 m lower than MHWS at Mallaig, but with a standard error of 0.54 m this reconstruction is the least precise. At 50 cm with an estimated RWL of 2.59 m OD Morar is the most accurate reconstruction, 0.21 m above MHWS at Mallaig and with the second smallest standard error of 0.26 m is more precise than the regional and Kintail training sets.

XY plots comparing the regional pollen reconstruction with the local reconstructions (figure 5.11) show the differences in the RWL estimates. The comparisons indicate that the regional training set consistently overestimates RWL in comparison to the Kintail and Morar training sets, whereas the Argyll training sets both over- and under-estimates RWL. Although the Kintail reconstruction consistently underestimates RWL it has the most linear relationship to the regional training set, mirroring the trends, but being slightly offset.

Table 5.1 shows that the regional pollen training set has the most modern analogues with 68.9 %, lower than the percentage of diatom modern analogues. Of the local modern training sets Argyll has the highest percentage of modern analogues. Table 5.2 shows that the pollen assemblages from the multi-proxy training set have slightly higher percentages of modern analogues, due to the reduced number of microfossils in the fossil core where samples in the fossil core are disregarded when both diatoms and pollen did not occur together.

5.3.3 Mointeach Mhor North multi-proxy reconstructions

The multi-proxy RWL reconstructions (figure 5.9) display a different trend to both the diatom and pollen only reconstructions. The multi-proxy reconstruction shows an unexpected gradual decrease in RWL to present and overestimates RWL in the organic silt-clay and the organic silt-clay with sand. The diatom and pollen only reconstructions both show a basic general trend of an increase in RWL in the organic silt-clay, followed by a decrease in RWL in the organic silt-clay with sand, and a gradual increase in RWL to present through the upper peat unit. Alternatively, the multi-proxy reconstruction shows the highest RWL is within the organic silt-clay, then the regional, Morar and Kintail all show a fall in RWL between 45 – 37 cm, indicating an increase in RSL, and RWL remains low until 20cm. Argyll departs from the other reconstructions at 41 cm when RWL increases to a peak at 36 cm indicating a fall in RSL in the organic silt-clay with sand. Then the Argyll reconstruction estimates a decrease in RWL between 36 – 32 cm. When comparing the reconstructions with the stratigraphic evidence, at 32 cm the reconstructions estimate RWL at 1.85, 1.95, 1.93 and 2.16 m OD respectively, with sample errors of 0.20, 0.33, 0.12 and 0.17 m OD. At 50 cm the reconstructions estimate RWL at 2.38, 2.59, 2.04 and 2.22 m OD respectively with sample errors of 0.23, 0.37, 0.13 and 0.18. At 32 cm the Argyll training set is most accurate, estimating RWL at 2.16 m OD, 0.22m below MHWS at Mallaig. At 50cm the regional training set is very accurate estimating RWL at 2.38 m OD, the same as MHWS at Mallaig, with a SE of 0.23 m.

XY scatterplots comparing the regional reconstruction with the local reconstructions for the pollen (figure 5.12) show the differences in the reference water level reconstructions. When comparing the diatom datasets figure 5.12 illustrates that the regional and Kintail RWL reconstructions produce the most similar RWL estimates.

Tables 5.1 shows that the regional multi-proxy training set has the most modern analogues, 78.5 % and the local training sets have percentages of modern analogues between 60 – 67.7 %.

Figure 5.13 compares the values of RWL (m OD) produced by the regional diatom, pollen and multi-proxy training set in turn. To allow direct comparison only the samples present in the multi-proxy training set were used. In addition, RWL reconstruction values could only be compared for depths within the core where both diatoms and pollen were recorded (20, 23, 26, 29, 32, 34, 36, 38, 41, 43, 45, 46, 47, 48, 49 and 50 cm) leaving 16 samples for comparison. This diagram was produced to allow comparison of the diatom, pollen and multi-proxy approach, using the regional datasets from monolith MMN01AB as an example. The diagrams illustrate that the diatom training set values of RWL are limited between 2.01 and 2.20 m OD and are not comparable with the pollen and multi-proxy estimates of RWL. The pollen has estimates of RWL between 1.42 – 4.21 m OD and the multi-proxy training set between 1.70 –2.41 m OD. The multi-proxy versus pollen diagram gives the most comparable estimates of RWL.

5.3.4 Mointeach Mhor North Summary

The diatom reconstruction produces a trend similar to expected when considering the stratigraphy and microfossil data. At 32 cm the Argyll reconstruction is the most accurate but is not the most precise with a standard error of 0.33 m. At 50 cm the Kintail dataset is the most accurate but with a standard error of 0.60 m is the least precise. At 32 and 50 cm the local training set from Saideal nan Ceapaich in Morar, although not providing the most accurate reconstruction, is the most precise and has the smallest associated standard errors of 0.19 and 0.25 m respectively. The RWL reconstructions containing just the diatom samples in the multi-proxy training also show an expected trend. At 32 cm the regional reconstruction is the most accurate only 0.2 m below MHWS at Mallaig, with a SE of 0.23 m. Whereas in the peat at 50 cm the Kintail RWL reconstruction is most accurate but with a standard error of 0.38 m is the least precise. The local Morar training set reconstructions at 32 and 50 cm have standard errors of 0.13 and 0.14 m respectively, and are once again the most precise. Morar is the most precise at both 32 and 50 cm as it has the smallest associated standard errors. Kintail is the most accurate at 50 cm, but the diatoms from the multi-proxy training set were most precise. At 32 cm the original diatom dataset from Argyll is the most accurate, but the diatom reconstruction using diatoms from the multi-proxy training set indicate that the regional reconstruction is the most accurate.

Neither pollen RWL reconstructions show a trend synonymous with the microfossil and stratigraphic data and the different dataset reconstructions are clearly affected by the length of the environmental gradient over which the modern samples were taken. For the original diatom dataset at 32cm Kintail is most accurate but has the joint second largest standard error. At 50 cm the Argyll reconstruction is most accurate but has the second largest standard error of 0.82 m. At 32cm the pollen dataset containing only the samples within the multi-proxy training set Kintail is the most accurate estimate, 0.12 m lower than MHWS at Mallaig, but with a standard error (SE) of 0.54 m this reconstruction is the least precise. At 50 cm the Argyll pollen reconstruction with a standard error of 0.23 m is the most precise. At 50 cm the local Morar reconstruction is the most accurate, 0.21 m above MHWS at Mallaig and with the smallest standard error of 0.27 m is the most precise. Identical to the diatom reconstructions the Morar training set is most precise at both 32 and 50 cm. At 32 cm the Kintail datasets are most accurate, but the pollen from the multi-proxy dataset from Kintail is most precise. At 50 cm the original Argyll diatom dataset is the most accurate but the multi-proxy pollen reconstruction for Morar is the more precise.

The multi-proxy reconstruction shows a gradual decrease in RWL, or decrease in RSL to present and overestimates RWL in the organic silt-clay and the organic silt-clay with sand. At 32 cm the Argyll training set is most accurate with the second smallest standard error of 0.17 m, here the Morar training set is most precise with a SE of 0.12m. At 50cm the regional training set is very accurate estimating RWL at 2.38 m OD, the same as MHWS at Mallaig, but has the third largest standard error of 0.23 m, once again at this point the point the Morar reconstruction is most precise with a SE of 0.13 m.

For core MMN01AB the multi-proxy training set has the most modern analogues within the fossil monolith (78.5 %). The diatom and pollen training sets taken from the multi-proxy training set have 73.1 and 73.8% modern analogues, slightly less than the original multi-proxy training set.

5.4 BARR-NA-CRICHE

Core BC006a from Barr-na-Criche in Knapdale is the most southerly fossil core and only preserves pollen microfossil data. Figure 5.14 shows the lithology, microfossil data and RWL reconstruction for core BC006a. This section reveals a minerogenic unit of organic silt-sand at the base of the core overlain by a peat. When considering the stratigraphical and microfossil evidence the reference water level reconstruction should have assemblages indicative of a salt marsh community in the basal minerogenic unit at lower RWL values grading into a freshwater alder carr community with an increase in RWL indicating a decrease in RSL. The microfossil evidence corroborates the stratigraphic data. Between 68 – 60 cm the pollen assemblages are dominated by gramineae and salt marsh indicator species, for example, *Plantago maritima*. At 60 cm and above there is a change from salt marsh pollen assemblages to taxa indicative of a freshwater alder carr environment, dominated by *Alnus*, with *Betula* and *Cyperaceae*, typical of a wet woodland habitat.

5.4.1 Barr-na-Criche pollen reconstruction

The regional, Morar and Argyll pollen RWL reconstructions do not estimate the RWL as expected, with RWL fluctuating slightly, with no specific trend.

Alternatively the Kintail pollen RWL reconstruction does estimate a trend synonymous with the stratigraphic and microfossil evidence, with low RWL estimates in the minerogenic unit between 68 – 60 cm and an increase in RWL in the overlying peat unit indicating a fall in RSL. To test the reliability of the estimates comparisons of the estimates in RWL can be compared with MHWS at the nearest tidal gauge at East Loch Tarbert (1.78 m OD) where peat formation commences. At 60 cm where peat formation begins the RWL estimates for the regional, Kintail, Morar and Argyll reconstructions are 2.62, 3.01, 1.88 and 2.20 m OD respectively, with associated errors of 0.52, 0.90, 0.30 and 0.49 m OD. Therefore at this point Morar is the most accurate reconstruction estimating RWL at 1.88 m OD, 0.10m above MHWS at East Loch Tarbert.

XY scatterplots comparing the regional and local pollen reconstructions (figure 5.15) illustrates that all of the datasets have very differing estimates. The Kintail reconstruction both over- and under-estimates RWL in comparison, which can be clearly seen on figure 5.14 where it has lower RWL reconstructions in the organic sand-silt, and over-estimates in the peat. The Morar reconstruction consistently under-estimates RWL, the Argyll reconstruction also under-estimates RWL but produces estimates most similar to the regional reconstruction.

Tables 5.1 shows that the regional pollen training set has the most modern analogues, 76.2 % and that the local training sets have the same percentages of modern analogues 71.4 %, although they are not necessarily the same species within the 71.4 % of modern analogues.

5.4.2 Barr-na-Criche Summary

The microfossil data at Barr-na-Criche is limited as only pollen is preserved in the fossil core; it is in these circumstances that the ability to apply a multi-proxy transfer function would be most useful. However, this only allows comparison of the training sets from different locations, not comparison between different microfossils. It is only possible to summarise by noting that the Morar reconstruction is most accurate where peat formation commences and with the smallest errors is also the most precise, although it is the Kintail pollen reconstruction that produces trends of RWL most synonymous with the stratigraphic and microfossil data.

The regional pollen training set has the most modern analogues, 76.2 % and that the local training sets all have 71.4 % modern analogues.

5.5 SUMMARY

For each fossil reconstruction the local Morar training set always proved to be the most precise as it consistently had the smallest sample-specific standard errors. This has implications for other research at it implies that a small local training set produces more precise estimates of RWL than large regional training sets.

However when the reliability of the transfer functions was compared to the stratigraphy, microfossils and local tidal predictions the original training sets containing all of the available samples proved more accurate than the training sets using just the diatom or pollen samples present in the multi-proxy training sets. The implications of these findings, problems with the methodology and future research will be discussed in Chapter 6.

Chapter 6 Discussion

6.0 INTRODUCTION

This chapter discusses the success of the microfossil-based transfer function (TF) reference water level (RWL) reconstructions on the west coast of Scotland to answer the research questions set out in section 2.1. This chapter also discusses what affects the success of the TF technique and what its limitations are, considers the implications of this research, and considers further research that could be carried out to improve the TF reconstruction precision and reliability.

6.1 WHICH TRANSFER FUNCTION MODELS DEMONSTRATE THE BEST PERFORMANCE DIATOM, POLLEN OR MULTI-PROXY?

6.1.1 Performance of the transfer functions

To allow comparison with other studies and to make the RMSEP values more meaningful the RMSEP values have been back transformed from SWLI units into m OD. Table 6.1 summarises the statistical parameters for each of the chosen transfer function models in Chapter 4. Table 6.2 summarises the same information for the training sets that contain the multi-proxy training sets and the diatom and pollen training sets that only comprise the samples in the multi-proxy training sets. The RMSEP values have been converted to m OD for each of the fossil sites at Nonach, Mointeach Mhor North and Barr-na-Criche taking into account local tidal parameters and displayed to the right of the tables. This allows comparison of the errors associated with the diatom, pollen and multi-proxy reconstructions, although when the reconstruction (calibration) is carried out there will also be additional errors associated with the goodness of fit. These RMSEP values also allow comparison of the prediction errors of other research.

The regression process and the resultant statistical parameters produced indicate that the multi-proxy training sets are most precise as they have the highest r^2 values, with the exception of the Argyll diatom training set with an r^2 value of 0.97 which statistically performed better than the Argyll multi-proxy training set. All of the multi-proxy training sets had lower RMSE and RMSEP values than the diatom and pollen training sets, but when a method of cross validation was applied the resultant $r^2_{(boot)}$ and $r^2_{(jack)}$ values were higher for the diatom training sets than for the multi-proxy training sets (Table 6.1). These results suggest that after cross validation the diatom training sets have potentially got better predictive capabilities than the multi-proxy training sets, but the multi-proxy training sets have smaller associated errors. The diatom training sets perform almost as well as the multi-proxy training sets and the pollen training sets are the least precise, for example, the regional pollen training set has RMSEP values equivalent to 1.18, 1.07 and 0.75 m OD for Nonach, Mointeach Mhor North and Barr-na-Criche respectively. Table 6.1 indicates that the precision of the transfer functions increases further when only diatom or pollen samples that were present in the multi-proxy training set are used. The Morar training set performs best for the diatom, pollen and multi-proxy transfer functions despite comprising only 22 diatom samples, 15 pollen samples and 15 multi-proxy samples, and performs best for the training sets containing only the samples in the multi-proxy training set that comprise 15 samples each. The results of the Canonical Correspondence Analysis suggest that the diatoms and pollen from Saideal Ceapaich in Morar have a very good statistical relationship with their associated environmental variables which explain 51, 53 and 43 % of the variance in the training sets for the diatom, pollen and multi-proxy training sets respectively. This statistically strong relationship appears to have a positive impact on the predictive capabilities and precision of the training set.

Very few published studies give the RMSEP value after cross validation, Sawai *et al.* (2004) give a $RMSEP_{(jack)}$ value of 0.29. The Morar diatom and multi-proxy transfer functions in this study have comparable $RMSEP_{(boot)}$ values to that published in Sawai *et al.* (2004) (Table 6.1) where a transfer function was successfully applied to fossil data, but the other transfer function models have higher RMSEP values.

To summarise, the multi-proxy training sets have the best performance as they have the highest r^2 values and are most precise because they have the lowest RMSEP values. The local Morar multi-proxy training set demonstrates the best transfer function model performance closely followed by the Morar local diatom training set and the RMSEP values for these transfer functions are comparable to those of other studies (e.g. Sawai *et al.*, 2004). With r^2 values of 0.99 and 1.00 respectively, their performance is exceptionally good. When the multi-proxy training set is compared to the diatom and pollen training sets with only the samples included in the multi-proxy training set for direct comparison the Morar local diatom transfer function performs best of all as it has a lower RMSEP value than the multi-proxy training set and the r^2 same value ($r^2 = 1.00$).

Although the multi-proxy transfer functions appear to perform very well it must be noted that the multi-proxy training sets do not contain as many samples as the diatom or pollen only samples. For example, the regional diatom training set contains 116 samples, whereas the multi-proxy training set contains only 75 samples, as does the diatom training set containing samples from the multi-proxy training set. As a result these training sets contain 41 samples less than the regional diatom training set, this may have an impact on the predictive capabilities of the training set when applied to the fossil samples as it will reduce the chances of the fossil data having suitable modern analogues.

Indeed comparison of the RWL reconstruction values for the regional diatom, pollen and multi-proxy training sets using only the samples present in the multi-proxy training set (Chapter 5, Figure 5.13) indicate that the predictive capabilities of the training set is compromised by using training sets containing less samples. In this instance the estimates of RWL originating from the regional diatom training set are very limited and are unable to reconstruct RWL values above MHWS. The regional pollen training set provides the highest estimates of RWL when compared to both the diatom and multi-proxy training sets, whereas unsurprisingly the multi-proxy training set provides higher estimates of RWL than the regional diatom training set but lower than the regional pollen training set. All of the training sets utilising only the samples in the multi-proxy training set provided unreliable estimates of RWL, this is probably because using less samples means that the training sets are not as statistically robust. This indicates the reconstructions are more vulnerable to the problems associated with the transfer function methodology, such as no analogues, multiple-analogues and the influence of allochthonous species as detailed in section 6.4.

6.2 WHEN COMPARING REGIONAL VERSUS SITE-SPECIFIC TRANSFER FUNCTION MODELS, WHICH RECONSTRUCTIONS PROVIDE THE MOST ACCURATE AND PRECISE RECONSTRUCTIONS?

In Chapter 4 the performance of the transfer functions was assessed by looking at the statistical parameters produced, and in Chapter 5 the performance of the RWL reconstructions was assessed for the various training sets by comparing the results with the stratigraphy, bio-stratigraphy and local tidal data. In this chapter it must be determined whether this method proves to be a viable option to reconstruct RWL and whether local or regional training sets estimate RWL most accurately and precisely.

To simplify the discussion monolith MMN01A & B will be used as an example to discuss and evaluate the performance of the diatom, pollen and multi-proxy reference water level (RWL) reconstructions (figures 6.1 – 6.3). It is also possible to compare the transfer function inferred RWL estimates with the published results of Shennan *et al.* (2005), where the same microfossil data was used to produce four sea-level index points. Each sea-level index point has an indicative meaning comprising a reference water level and an error term. The reference water levels and error terms associated with the sea-level index points can be compared with the results of the diatom, pollen and multi-proxy RWL reconstructions at the same (or similar) depths within the fossil sample. This will give an indication of how the transfer function inferred estimates compare with the published RWL estimates for the four sea-level index points.

6.2.1 Diatom RWL reconstructions

The diatom RWL reconstructions to consider are shown in figure 6.1. The most useful RWL reconstruction to assess is the RWL reconstruction at the far right of the diagram utilising diatom samples from the multi-proxy training set, as this reconstruction allows direct comparison of the RWL reconstruction produced by the multi-proxy training set (figure 6.3). It appears that the diatom training sets only utilising diatom samples occurring in the multi-proxy training set do not have the ability to infer RWL values above MHWS in the upper peat (Tables 6.4 & 6.5). Even though the statistical parameters produced in Chapter 4 suggest that the training sets containing the diatom samples present in the multi-proxy training set are the most precise and have the best predictive capabilities these reconstructions must be deemed unreliable.

The original diatom training sets provide RWL estimates similar to what one would expect considering the bio-stratigraphy, lithology and local tidal data. Table 6.4 allows comparison of the RWL estimates calculated using the transfer function technique with the estimates of RWL for the nearest sea-level index (SLI) point. As the SLI point is at 33 cm, the transfer function based estimates from 32 and 34 cm must be compared with the SLI point. At 32 cm the Argyll training set was most accurate estimating RWL at 2.32 m OD, 0.06 m above MHWS at Mallaig, a more accurate estimate than the SLI point, but with errors of 0.33 m is less precise. At 34 cm the Morar training set is most accurate estimating RWL at 2.32 m OD, 0.06 m above MHWS at Mallaig, but with errors of 0.17 m is both more accurate and more precise than the SLI point when compared to the tidal data. At 46 cm and 50 cm the Argyll training set gives estimates closest to the SLI point RWL estimates but has much larger errors. So the diatom-based transfer function RWL reconstructions give estimates of RWL comparable to the information provided by the SLI points at four places in the core, but how reliable are the diatom-based RWL reconstructions throughout the monolith sample? The regional and Morar diatom training set reconstructions reflect the expected pattern of RWL with a peak of marine influence in the organic silt-clay with sand and a gradual increase in RWL to present. The Kintail RWL reconstruction consistently under estimates RWL from 40 cm to present and the Argyll training set fluctuates between over and under-estimating RWL and indicates an increase in RWL in the organic silt clay with sand. The Argyll training set RWL reconstruction is most accurate when compared to the tidal data and SLI points at 32, 46 and 50 cm, but like the Kintail training set produces erroneous estimates of RWL in the organic silt-clay with sand. It appears that either the Morar or regional RWL reconstruction could give additional information on the timing and elevation of RWL during the mid-Holocene high stand and have the potential to produce a sea-level curve of RWL for this section of the fossil monolith sample.

6.2.2 Pollen RWL reconstructions

The pollen-based transfer function RWL reconstructions (figure 6.2) do not show a synchronous trend with the microfossil and stratigraphic data and the Argyll training set produces rather high RWL estimates, which in turn affects the regional reconstruction suggesting that the length of the environmental gradient over which the training set samples are collected influences the inferred RWL values. Table 6.1 shows that the RMSEP values once converted into m OD represent substantial reconstruction errors, with only the Morar pollen training set having errors less than 0.5 m. When considering that the difference between the MTL and MHWS at Mallaig is 2.1 m, 0.5m is almost a quarter of the difference between MTL and MHWS. The pollen transfer function performance statistics attribute the Kintail training set with a $\text{RMSEP}_{(\text{boot})}$ value of 1.34 m OD, over half the difference between MTL and MHWS. Tables 6.2 and 6.5 indicates that for the regional pollen training set these values are approximately halved when the only the samples in the multi-proxy training set are used. So which pollen training sets give the most sensible estimate of RWL and are most accurate and precise?

At 10 cm the Morar pollen training sets produces a RWL most similar to the SLI point, but is 0.8m below the SLI point inferred RWL and the regional, Kintail and Argyll are all over-estimating. At 32cm and 34 cm the Kintail RWL reconstruction is most similar to the SLI point inferred RWL reconstruction and the predicted MHWS at Mallaig. At 32 and 34 cm Morar has the smallest sample errors making it most precise. At 50 cm the Argyll reconstruction is the most accurate at 2.57 m OD, 0.19 m OD below MHWS at Mallaig and is nearest to the SLI point inferred value of RWL (2.28 m) but the local training set from Morar, with a SE of 0.38 m provides the most precise reconstruction.

The pollen training sets containing only the samples within the multi-proxy training set, at the far right of figure 5.8, also display a similar trend to the dataset with all available samples, although the fluctuating estimates of RWL in the minerogenic units are surprisingly more pronounced and still the opposite of what one would expect. At 10cm the Argyll training set is the most accurate compared to the SLI point, but the Morar training set is the most precise. At 32 cm the Kintail training set is the most accurate but the Argyll training set is the most precise. At 46 and 50 cm the Morar training set is the most accurate and is the most precise. The regional pollen inferred RWL reconstruction estimates RWL lower than the training set containing all available samples. None of the pollen RWL reconstructions provide sensible estimates of RWL throughout the monolith sample and if the results were taken on face value without considering the stratigraphy they would produce an erroneous record of RWL as the poor performance of the transfer function is reflected in the unreliable RWL reconstructions.

6.2.3 Multi-proxy RWL reconstructions

The multi-proxy-based transfer function results indicated that multi-proxy training sets (table 6.4) generally performed better than the pollen and diatom only transfer functions and produced the most precise reconstructions. However, the excellent statistical parameters produced by the regression process are not reflected in the RWL reconstruction when the multi-proxy training sets are used to calibrate the fossil data. The multi-proxy RWL reconstructions (figure 6.3) display a peak of RWL in the organic silt-clay, then correctly estimate lower RWL within the organic silt-clay with sand, but then only the Argyll training set is capable of estimating RWL above MHWS once peat formation commences, but the Argyll training set training set also estimates a peak of RWL in the organic silt-clay with sand. This indicates that the multi-proxy reconstructions are unreliable as they under-estimate RWL in the upper peat and over-estimate RWL in the organic silt-clay and the organic silt-clay with sand.

The transfer function-based RWL reconstructions can now be compared with RWL estimated of the SLI points produced by Shennan *et al.*, 2005. At 32 and 34 cm the Argyll training set gives values closest to the SLI point inferred RWL at 32 cm but the transfer function based RWL reconstructions are under-estimating RWL at this point. At 46 cm the Kintail and Morar training sets are producing comparable estimates of RWL, and the Morar training set has an associated error of just 0.13 m, which is more precise than the SLI point. At 50 cm the Argyll multi-proxy training set just 0.06 m below the SLI point inferred RWL. This result indicates that the multi-proxy training set performs well apart from in the peat where the estimates of RWL are under-estimated.

6.2.4 Summary- which reconstructions are the most accurate and the most precise local or regional?

For the diatom inferred RWL reconstructions the Argyll training set RWL reconstruction is most accurate when compared to the tidal data and SLI points at 32, 46 and 50 cm, but like the Kintail training set produces erroneous estimates of RWL in the organic silt-clay with sand so there are doubts about its reliability. The Morar training set is the most accurate at 34 cm and is the most precise throughout the monolith.

For the pollen inferred RWL reconstructions the pollen transfer function inferred RWL reconstructions utilising only the samples in the multi-proxy training set have the best transfer function performance, however the reconstructions are rather unreliable. There is no one training set that gives a sensible reconstruction. At 10cm the Argyll training set is the most accurate compared to the SLI point, but the Morar training set is the most precise. At 32 cm the Kintail training set is the most accurate but the Argyll training set is the most precise. At 46 and 50 cm the Morar training set is the most accurate and is the most precise.

At 32 and 34 cm the Argyll training set gives values closest to the SLI point inferred RWL but the transfer function based RWL reconstructions are under-estimating RWL at this point. At 46 cm the Kintail and Morar training sets are producing comparable estimates of RWL, and the Morar training set has an associated error of just 0.13 m, which is more precise than the SLI point. At 50 cm the Argyll multi-proxy training set just 0.06 m below the SLI point inferred RWL. The Morar training set is the most precise throughout.

The statistical parameters produced after regression suggests that the Morar training sets are the most precise. The Morar multi-proxy training set is most precise, closely followed by the Morar diatom training set that only contains the samples in the multi-proxy training set.

6.3 CAN MULTI_PROXY TRANSFER FUNCTIONS RECONSTRUCT REFERENCE WATER LEVELS MORE PRECISELY?

Statistically the multi-proxy training sets have the potential to reconstruct RWL more precisely than training sets containing only one microfossil. In this research the original training sets containing all available samples gave more sensible and reliable estimates of RWL than the multi-proxy samples which contained fewer samples.

A transfer function model with a relatively low RMSEP value and high r^2 value is only useful to reconstruct RWL if it provides modern analogues for the fossil data, so there is a trade off between the model being precise and being widely applicable. This is the case in this study as the statistical parameters produced as a result of regression suggest that the multi-proxy transfer functions, and the diatom and pollen training sets that only contain the samples within the multi-proxy training set, will perform best. In reality when the training sets are used to calibrate the fossil data the original training sets with all available samples may not be as precise, but the inferred estimates of RWL are more reliable.

6.4 PROBLEMS ASSOCIATED WITH TRANSFER FUNCTION INFERRED RWL RECONSTRUCTIONS

There are a number of problems associated with the transfer function technique and the effect this can have on the resultant estimations of RWL. These include problems associated with screening the data, spatial autocorrelation, under- and over-estimation of RWL, no analogue situations, multiple analogues, allochthonous / autochthonous species, secondary environmental gradients and problems with the sampling strategy.

6.4.1 Screening the data

In an attempt to improve precision many authors screen the biological data after regression has been carried out to remove samples or species that have the potential to produce erroneous reconstructions (e.g. Fritz *et al.*, 1991; Gasse *et al.*, 1995; Zong & Horton, 1999; Edwards *et al.*, 2004). A large heterogeneous dataset will inevitably contain some samples that do not have a good statistical relationship with one or more of the environmental variables being investigated due to the influence of other environmental variables, taphonomic issues, natural variability or human error. Martens and Naes (1989) suggest that such outliers can decrease the predictive ability of the estimated transfer function coefficients and that these outliers should be identified and removed from the dataset. Data is screened in a variety of ways, Gasse *et al.* (1995) initially removed species that were only present in one sample, or had a maximum relative abundance of less than 1% and after derivation of initial transfer functions they removed further samples that had a difference between the observed and jack-knife-inferred environmental value of greater than one quarter of the total range; Zong & Horton (1999) followed the methodology of Fritz *et al.* (1991) and only used taxa that reached 5% of the total sum; Edwards *et al.* (2004) removed species contributing less than 2% of the total.

Although there is obviously some general agreement that screening the data is statistically acceptable, from an ecological perspective it is difficult to ascertain why this is considered a valid method. In this research all samples and species (simply converted into percentages) available were utilised, as the main function of the training set is to provide as many different assemblages from a variety of habitats to increase the chances of finding samples that are representative of the fossil assemblages. Thus, screening of the data appears to do just the opposite. Indeed Birks (1998) surprisingly reported that recent studies have highlighted that inference models based on either WA or WA-PLS with the lowest RMSEP and bias are invariably the models that are based on all taxa (Birks, 1994; Wilson *et al.*, 1996; Cameron *et al.*, 1999) even though many of the taxa only occur 1-3 times in the training set. This conflicts with statistical expectations, possible explanations could be that the estimated WA-PLS coefficients of very rare taxa are contributing some ecological information to the inference model rather than having no effect or detrimentally introducing statistical noise or random variation into the model (Birks, 1994). This suggests that screening the data, rather than removing samples or species that have the potential to produce erroneous reconstructions could actually remove valuable ecological information and reduce the predictive capabilities of the training set. The implication is that the more samples a training set contains the better, as the inferred RWL values will be more accurate and precise.

6.4.2 Spatial autocorrelation

Another problem associated with the transfer function technique is the consideration of spatial autocorrelation. One of the main assumptions in the use of transfer functions is that the environmental variable of interest is, or is highly correlated with, an ecologically important variable (Birks, 1995). This suggests that it should not be possible to reconstruct variables of no ecological importance. If the training set comes from sites that are independent a model with no predictive power would be expected to have an r^2 value near zero. However, if the sites are not independent due to spatial autocorrelation in the training set this can have implications. Telford *et al.* (2004) and later Telford and Birks (2005) suggest that spatial autocorrelation seriously violates the assumption that the test sites (training sets) are independent of the modelling sites. The predictive power of transfer functions assumes that the test sites are independent of the modelling sites. Cross validation in the presence of spatial correlation violates this assumption and the results are artificially high r^2 values. This theory may present a problem in this piece of research as the modern training set samples were on two occasions taken in close proximity to the fossil samples, the most obvious examples being Nonach and Barr-na-Criche where spatial autocorrelation may result in artificially high r^2 values, suggesting that the predictive capabilities of the local training sets was better than it actually was. The effects of these problems must be considered when the modern biological data is calibrated with the fossil data.

6.4.3 Over- and under-estimation of optima

Birks (1995) suggested that the two main reasons WA-PLS outperforms WA was that WA suffers from edge effects, therefore overestimating optima at the low end and under-estimating optima at the high end of the environmental gradient. For example, Gonzalez-Donoso *et al.* (2000) found that the TF technique over-estimated summer and winter sea surface temperatures at lower temperatures and under-estimated temperature at higher temperatures. Secondly, the influences of additional environmental variables to those of interest are ignored in WA even though they are likely to affect the composition and abundance of biological data. WA-PLS overcomes this problem with a process involving a weighted inverse deshrinking regression (ter Braak and Juggins, 1993) that tends to pull the inferred values towards the mean of the training set, but it does not completely remove the source of bias (ter Braak and Juggins, 1993; Lotter *et al.*, 1997, 1998) so there is still over-at low values and under-estimation at high values especially over long environmental gradients. This is evident when looking at the residuals of, for example, the regional diatom training set (figure 4.3) where there is a still a definite trend in the residuals, even though this model has reduced some of the trend in the residuals. This trend, or bias in the residuals may be caused partly by edge effects and partly as a result of other problems such as allochthonous species, and multiple analogues.

6.4.4 No analogues

No analogues situations occur when none of the modern training set assemblages are very similar in species composition and relative abundance to the fossil assemblages Birks (1998). However Birks (1998), found that WA-PLS performed surprisingly well in such cases as the transfer function technique tends to extrapolate. However, Gonzalez-Donoso *et al.* (2000), whilst studying MAT and TF to reconstruct winter and summer sea surface temperature using foraminifera transfer functions, found that non analogue situations can be a problem even if the species is present in both the fossil and model sample. This occurs if there are fossil samples in which the percentage of a particular species exceeds the maximum percentage recorded in the training set, and these samples are still to be considered as not possessing a biological analogue. For example, in the regional diatom training set (figure 4.1) the relative abundance of *Diploneis interrupta* does not exceed 20% of the total, but in the fossil assemblages at Mointeach Mhor North *Diploneis interrupta* reaches relative abundances of almost 60%, so even though they are present in the modern and fossil samples the training set assemblages will not be considered as a biological analogue. The pollen data has similar problems; the regional pollen training set contains assemblages where Cyperaceae pollen reach relative abundances of 50 %, but the fossil assemblages do not exceed 20% of the total.

Additional problem associated with pollen are that firstly, there is a wide variety of types/classifications of maritime vegetation that can potentially occur at any given tidal range (Rodwell, 1997) which may mean that pollen does not constrain sea-level tightly enough, especially at the high marsh or that a high marsh assemblage may not be present in the modern training set samples. Secondly, many contemporary marshes have differing salt marsh plant assemblages from those seen in Holocene sequences. This may be due to anthropogenic factors such as different intensities of grazing (e.g. Shennan *et al.*, 1995) and could cause non-analogue situations. Thirdly pollen can also have a patchy distribution and is not suited to clastic lithofacies, this is particularly a problem as there are no pollen producing (angiosperm) plant species on mudflats.

6.4.5 Multiple analogues

ter Braak *et al.*, (1996) discovered the effect multiple-analogues could have where the fossil assemblage is similar to several modern samples that differ widely in their environment. This is a particular problem in palynology, particularly when only a small number of pollen taxa of coarse taxonomic rank are used in calibration. The identification key for pollen types is sometimes too coarse, for example, it is not possible to distinguish between different

Cyperaceae and Gramineae types and also the differentiation in the genera of Chenopodiaceae and Asteraceae is restricted (Freund *et al.*, 2004).

Commonly high values of taxa such as *Pinus* or Gramineae can clearly be derived from a wide range of modern environments. For example, it is impossible differentiate between saltmarsh grass (*Pucinellia maritima*) on the low marsh and red fescue (*Festuca rubra*) on the high marsh. This problem is evident in figure 6.2 where high relative abundances of gramineae in the organic silt-clay and again in the upper peat layer causes the pollen training set RWL reconstructions to infer an similar estimates of RWL when the stratigraphy would indicate that there should be a lower RWL estimate in the organic silt clay. This is as a result of two considerations, pollen analysis is not suited to clastic facies as pollen bearing species do not grow on tidal flats, so this assemblage must be allochthonous. Secondly, this may be the grass pollen of saltmarsh grass but as the taxonomy is too coarse the model is treating it as grass pollen from the upper marsh as they have similar relative abundances. This is also linked to the problem of over and under-estimating optima where allochthonous or indistinguishable species create multiple analogues and introducing bias into the data.

6.4.6 Allochthonous and autochthonous species

Diatoms are regarded as very sensitive indicators of environmental change for a variety of environmental variables. However, one of the main challenges in marine diatom research is the problem in distinguishing between autochthonous and transported, allochthonous species in tidal and estuarine environments (Simonsen, 1962; Zong, 1997, Zong & Horton 1999). Sherrod (1999) stated that the main taphonomic processes that act on diatoms in salt marshes are transportation (e.g. Vos and De Wolf, 1993), breakage and dissolution (e.g. Denys, 1991/2; Ryves *et al.*, 2001). These processes can act alone or together altering the in-situ (autochthonous) diatom assemblages of a salt marsh resulting in species being either selectively removed from an assemblage by breakage or dissolution, or added by tidal current transport. Denys (1994) stated that relying on the presumed autoecology of individual species without giving due thought to the processes that produced the diatom assemblages (thanatocoenoses) can lead to erroneous interpretations. This is a very important consideration as assemblages may be either totally destroyed, or in cases of incomplete dissolution, the differential dissolution of the diatom valves and taxa may bias the composition of the assemblages within a sample and thus affect environmental inferences.

Sawai (2001) showed that *Paralia sulcata* and *Cocconeis scutellum* could be a significant allochthonous component in tidal marsh deposits. These two species are particularly problematic; living *Paralia sulcata* specimens form long chains (Crawford, 1979) and these chains can float and are transported on the tide and small specimens can be trapped on the ebb (Hemphill-Haley, 1995; Nelson & Kashima, 1993; Denys, 1999; Sawai, 2001; Sawai 2002). Sawai (2004) suggested that *Cocconeis scutellum* can also make a significant contribution to the allochthonous component of an assemblage, this epiphytic species lives attached to seaweed (e.g. fucoid algae), and living specimens are strongly attached by the Rapid valve (R-valve) even after death the Rapid valve remains attached to the seaweed with mucilage whereas separated P-valves are transported over long distances by the tidal currents. Therefore R-valves are often deposited at the strand line at MHWS on detached seaweed, whereas P-valves are entirely and selectively distributed on tidal environments, although its true habitat is limited to the seaweed zone. Figure 5.1 in Chapter 5 clearly illustrates the effect an allochthonous species such as *Cocconeis scutellum* can have on a reference water level (RWL) reconstruction. At 40 cm in the peat indicative of a tidal marsh community there is a large peak in the relative abundance of *Cocconeis scutellum*. The high relative abundance is then analogous to samples taken from low marsh environments thus giving a much lower estimate of RWL than expected, as the peat forming community would be expected to occur at MHWS or above. Allochthonous species are also evident in the fossil assemblage at Mointeach Mhor North where several freshwater species are recorded in the organic silt-clay, for example, *Tabellaria fenestrata*. These freshwater diatoms occur in the organic silt-clay due to bio-turbation, where they may have originated from the basal peat, or these freshwater diatoms may have been transported by a saltmarsh creek.

Pollen assemblages also have problematic species that contribute to the allochthonous component of an assemblage. One disadvantage of pollen is the wide dispersal of pollen types that are most buoyant in the air, which gives a misleading impression of the vegetation cover. *Plantago maritima* pollen grains are dominant in mostly all of the pollen counts of salt marsh deposits. However, the main distribution of the species is in the lower salt marsh vegetation zone (Freund *et al.*, 2004). Another problematic pollen type is *Pinus* as the pollen grains have an air sack to make them buoyant and they are commonly encountered on the tidal flats and lower marsh and are washed onto the marsh by the tide.

6.4.7 Secondary environmental variables

Secondary environmental gradients can be problematic at sites where the environmental variable that is being reconstructed is not the variable explaining most of the variance in the dataset (Birks 1995). However the results of Canonical Correspondence Analysis in Chapter 4 indicate that on only one occasion elevation (SWLI) is not the variable that explains most of the variance in the various training sets. At Saideal nan Ceapaich in Morar the percentage of sand is the variable explaining most of the variance closely followed by elevation (SWLI). However, whereas the influence of additional environmental gradients is ignored in WA, WA-PLS actually uses these interactions between the environmental variables to improve predictions so WA-PLS is not detrimentally affected by secondary environmental gradients (Juggins & ter Braak, 1997).

6.4.8 Statistical assumptions of the transfer function technique

For a unimodal transfer function to be able to efficiently estimate the optima of the diatom, pollen or diatoms and pollen in combination, a number of parameters must be met:

1. Diatom abundances are unimodal, the pollen abundances are linear and the multi-proxy abundances are unimodal (as applicable);
2. Sites are equally spaced over the whole range over which the taxa occur (Birks, 1995);

3. Taxa are not tightly clustered along the elevational gradient;
4. There is a fairly even turnover of species along the elevational gradient.

The problem with the sampling methodology used is that the samples are not evenly distributed along the environmental gradient. The difference in elevation between samples varies. The methodology did not aim for uniform sampling, but aimed to collect biological samples from a variety of modern samples to ensure that the samples represented the majority of local spatial variability within the full range of the environmental gradient sampled.

6.5 WIDER IMPLICATIONS OF THIS RESEARCH

The results of this research imply that multi-proxy transfer functions are more precise than diatom or pollen transfer functions. Also this research shows that diatom or pollen transfer functions utilising only samples present in the multi-proxy local training sets have higher r^2 and can be more precise than the training sets containing all available samples.

In addition the local training set from Saideal Ceapaich in Morar performed best having the lowest RMSE and RMSEP values and the highest r^2 value of the diatom, pollen and multi-proxy transfer function models (Tables 6.1 and 6.2).

These results have implications for other sea-level studies, as these findings suggest that a large modern training set may not be needed to calibrate a fossil core as a local training had the best transfer function performance, and that a local multi-proxy transfer function inferred estimates of RWL could be the most accurate and precise. So the question is, if a researcher has several fossil cores that they wish to use to reconstruct RWL using microfossil-based transfer functions and they are limited to using either a large regional training set from various samples along the coast or collecting samples from a limited number of local training sets what are the implication of these results.

The results of the regression indicate that a small local training set with a good statistical relationship with the environmental variables would be the best option to calibrate the fossil data and that a multi-proxy training set would produce the most precise results. Whereas in reality when the training sets were used to calibrate the fossil cores the original diatom training sets produced the most reliable estimates.

Another consideration is whether the statistical transfer function methodology yields any more information than the qualitative method of producing sea-level index points. A lot of emphasis is still placed on the need to evaluate and validate reconstructions. Birks (1998) suggested that there are still outstanding problems associated with transfer function models:

1) the need for a detailed and consistent taxonomy in the training sets
2) the quality, representativeness, and inherent variability of the environmental variables of interest
3) and the inherent bias in the calibration models.

Birks (1998) also suggested that having developed modern training sets, many palaeolimnologists are returning to the sedimentary record and are studying stratigraphical changes. To determine whether the transfer function methodology had any added value than collecting lots of stratigraphic samples for dating and microfossil analysis in section 6.2 the results of the transfer functions based RWL estimates were compared with the RWL values attributed to the SLI points produced by Shennan *et al.* 2005. The diatom training sets, in particular the Argyll training set, provided similar estimates of RWL to the SLI points and the local tidal and stratigraphic data and had the potential to yield additional information regarding the height of the mid-Holocene high stand. Whereas the pollen and multi-proxy based transfer function estimates were unreliable in the organic silt-clay with sand, as pollen analysis and thus multi-proxy analysis is not suited to these stratigraphic units.

It may be that the transfer function approach is not universally applicable. A lot of work has been done in recent years concerning the development of modern calibration data sets in palaeo-limnology to make down-core environmental reconstructions using a variety of biological proxies, but much work is needed to improve the ability to analyse stratigraphical data in terms of patterns, dynamics and rates of change. Perhaps the complexities of the tidal marsh assemblages and problems associated with and limitations of the transfer function technique indicate that the transfer function methodology is not the best method for RWL reconstructions on the west coast of Scotland. This does not mean that the technique is not valuable for other studies. Transfer functions have been successfully used in lots of other studies, for example, reconstructing sea surface temperature during the Quaternary using foraminifera-based transfer functions (Gonzalez-Donoso, 2000); inferring past hydro-chemical characteristics of African lakes using diatom-based transfer functions (Gasse *et al.*, 1995); reconstructing relative sea-level change using foraminifera-based transfer functions (Edwards & Horton, 2000; Edwards, 2001; 2004; Gehrels, 2000); using diatom-based transfer functions to provide evidence of earthquakes (Hamilton, 2005) (cycles of co-seismic land subsidence). These research projects were successful, so the transfer function technique should not be dismissed as unreliable until further research is carried out to improve the reliability of the reconstructions.

6.6 FURTHER RESEARCH

To try to improve the reliability of the RWL estimates it may be beneficial to collect more modern samples representative of the fossil environments to determine whether creating a larger regional dataset would provide more suitable analogues for calibrating the fossil data and improve the reliability of the RWL reconstructions. As it appears that the more samples a training set contains the more precise, accurate and reliable the inferred values of RWL will be. Expanding the training set to include more samples from a variety of tidal marsh habitats would be useful as one of the biggest limitations in quantitative palaeo-environmental reconstructions is the need for high-quality modern training sets of consistent and detailed taxonomy, comparable methodology and sedimentary environment.

In addition to expanding the modern training set it would also be very useful to either have each of the samples radiocarbon dated to produce sea-level index points or use a mathematical model to assign each sample with an age to enable the production of a sea-level curve. Production of an age-elevation plot using the transfer function inferred estimates of RWL would allow comparison with the age-elevation plot of sea-level index points published by Shennan *et al.* 2005 for the Arisaig area.

6.7 SUMMARY

This chapter discussed the success of the microfossil-based transfer function reference water level (RWL) reconstructions to answer the research questions set out in section 2.1. This chapter compared the transfer function inferred estimates of RWL with the RWL values of sea level index (SLI) points produced by Shennan *et al.* (2005). The problems and limitations of the transfer function technique and how they could have affected the transfer function based estimates of RWL Where also discusses. Finally, the implications of this research and further research that could be carried out have been considered.

Chapter 7 Conclusions

7.0 INTRODUCTION

This chapter concludes the thesis by assessing the extent to which the initial research aims and objectives outlined in chapter one have been met and to produce an outline of this research project and the key findings.

7.1 PROJECT SUMMARY

This study is a first attempt to develop transfer functions using three local modern diatom, pollen and multi-proxy training sets then in combination as large regional training sets. These transfer functions were then used to provide reconstructions of relative sea-level by applying the modern biological data to fossil datasets from Nonach, Mointeach Mhor North and Barr-na-Criche. This allowed comparison between the different microfossil reconstructions and those arising from regional versus site-specific transfer function models.

This research project aimed to answer three broad research questions:

1. Which transfer function models have the best performance, diatom, pollen or multi-proxy?
2. When comparing regional versus site-specific transfer function models, which reconstructions, local or regional, provide the most accurate reconstructions?
3. Can multi-proxy transfer functions reconstruct RWL more precisely and reduce the vertical error bars associated with RWL reconstruction?

These research questions were answered using the following approach:

a) Six modern field sites were selected on the west coast of Scotland, three sites from Kintail, one site from Morar and two sites on the Argyll coast provide the local training sets, and in combination form a regional training set. The samples came from a variety of habitats from the tidal flats to above the highest astronomical tide.

b) The diatom, pollen and multi-proxy training sets were studied to ascertain the relationship between the diatom, pollen and multi-proxy assemblages and a suite of environmental variables (pH, LOI, salinity, % sand, % silt and % clay). The subsequent results in Chapter 4 show that the distribution of the diatom, pollen and multi-proxy assemblages is usually a direct function of elevation, with the exception of the diatom assemblages at Morar where the distribution of the diatom taxa was a direct function of salinity, closely followed by elevation. The Morar training set assemblages had the most variance explained by the environmental variables.

c) The next stage was to investigate the quantitative relationship between the diatom, pollen and multi-proxy assemblages and elevation in order to develop transfer function models for reconstructing RWL. Comparison of the performance of the diatom, pollen and multi-proxy training sets was undertaken by comparing the performance statistics of the transfer function models. The performance statistics suggest that the precise reconstruction of RWL is possible, and that multi-proxy transfer functions are more precise than diatom and pollen training sets.

d) To ensure that the results were directly comparable and not just an artefact of sample size, the transfer functions were computed again to compare the regional multi-proxy training set to regional training sets comprising the diatom and pollen samples from the multi-proxy training set so that exactly the same samples, and same number of samples were used. The results indicated that the multi-proxy training set once again performs best, followed closely by the diatom training set. The pollen training set once again has the poorest performance.

e) In Chapter five these transfer functions provide reconstructions of RWL for fossil samples from Nonach, Mointeach Mhor North and Barr-na-Criche. These allow comparisons between the different microfossil reconstructions and those arising from regional versus site-specific transfer function based RWL reconstructions. To test the reliability of the RWL reconstructions each was assessed by comparing the results with the lithostratigraphy, the microfossil assemblages and the size of the associated errors. For Core NN04 at Nonach the regional multi-proxy reconstruction produces a reconstruction similar to what one would expect considering the stratigraphic and microfossil evidence. For monolith MMN01AB the diatom training sets containing all available samples produce a trend of RWL most similar to that suggested by the stratigraphic and bio-stratigraphic evidence. For core BC006a the Kintail pollen reconstruction estimates a trend in RWL very close to what one would expect when considering the stratigraphic and bio-stratigraphic evidence.

f) In Chapter 6 monolith MMN01A&B at Mointeach Mhor North was used as an example to discuss the success of the microfossil-based transfer function reference water level (RWL) reconstructions on the west coast of Scotland to answer the research questions set out in section 2.1. Factors, which affect the success of the TF technique, were discussed in addition to the limitations of the technique. The implications of this research were considered, and further research that could be carried out to improve the TF reconstruction precision and reliability. In Chapter 6 transfer function-based estimates of RWL were compared with the RWL estimates of the sea-level index points published by Shennan *et al.*, (2005).

The Argyll diatom training set RWL reconstruction proved to be most accurate when compared to the lithostratigraphy, tidal data and SLI points at 32, 46 and 50 cm, but like the Kintail training set produces erroneous estimates of RWL in the organic silt-clay with sand. It appears that either the Morar or regional diatom RWL reconstruction could give additional information on the timing and elevation of RWL during the mid-Holocene high stand and have the potential to produce a sea-level curve of RWL for this section of the fossil monolith sample.

Chapter 8 References

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