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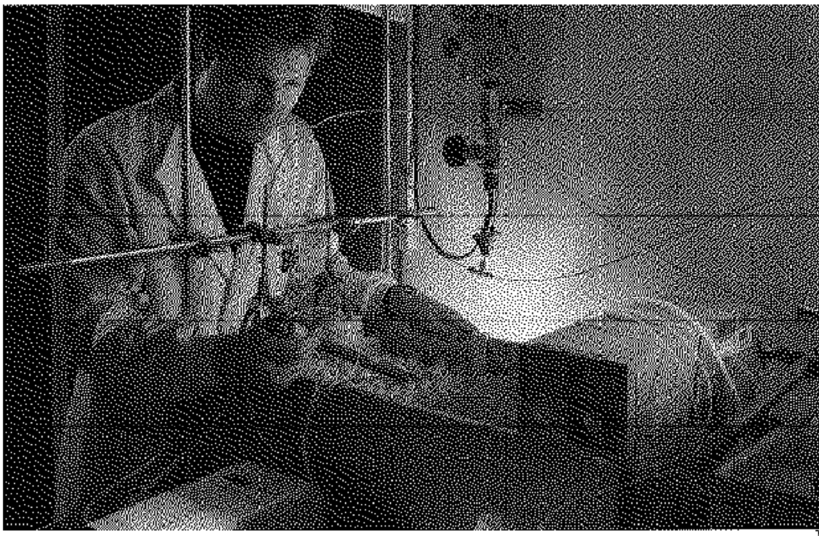
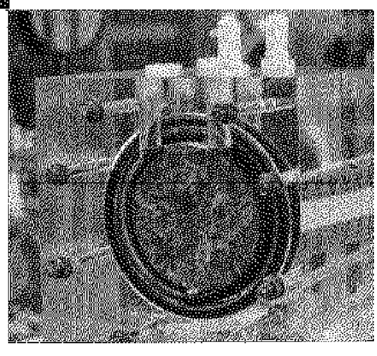
Science Report

Nirex Safety Assessment Research Programme



Nirex Biosphere Research: Report on Current Status in 1994



July 1995

NIREX

SCIENCE REPORT

Nirex Biosphere Research:

Report on current status in 1994

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PREFACE

Nirex is responsible for the development of a deep geological repository for the disposal of solid intermediate-level and some low-level radioactive waste. In 1991 an area near Sellafield, West Cumbria was chosen as the focus for further investigations following preliminary investigation of two sites. The Nirex Science Programme is directed at establishing the suitability, or otherwise, of the site at Sellafield to host the deep repository. This requires, amongst other things, that an assessment be developed of the post-closure performance of a repository located there and that this assessment should be supported by information from a suitably designed research programme.

The Nirex Safety Assessment Research Programme (NSARP) is a wide ranging programme providing detailed understanding and data on the physical, chemical and biological processes that may be of relevance to repository post-closure safety together with mathematical models describing the way that these processes operate and interact. The NSARP is principally concerned with improving our knowledge of two important pathways, groundwater and gas, through which radionuclides may return to the human environment and it is supplemented by a more engineering-orientated programme of research into the Nirex Reference Vault Backfill.

Current Status Reports are intended to provide an overview of the research programme and so help to document its development. They rely on detailed information contained in Nirex reports and other documents in the public domain. The Nirex reports referred to here are mostly Nirex Safety Series (NSS) reports or the Nirex Science reports that have been introduced recently. All these reports have been produced by contractors partly or fully funded by Nirex and working under Quality Assurance arrangements which are either in strict accordance with BS5750 or, particularly for some of the earlier reports, in keeping with its intent.

1 Introduction

Nirex is responsible for the development of a deep geological repository for the disposal of solid intermediate-level and some low-level radioactive wastes (ILW and LLW respectively). In 1991 an area near Sellafield, West Cumbria was chosen as the focus of further investigations, following preliminary geological investigations of two sites. The Nirex Science Programme is directed at establishing the suitability, or otherwise, of the site at Sellafield to host the deep repository. This requires, among other things, that an assessment he developed of the post-closure performance of a repository located there.

The Nirex Disposal Safety Assessment Team (DSAT) has been developing post-closure performance assessments in a progressive manner, as an increasing amount of information has become available. The main sources of information are the Site Characterisation Programme, which delivers information about the surface and subsurface characteristics of the potential site, and the Nirex Safety Assessment Research Programme (NSARP), which delivers information concerning the fundamental physical, chemical and biological processes affecting the safety programme. Modelling and methodological developments within the NSARP are used either directly in assessments or to help develop understanding of the system. The NSARP is divided into four broad sectors relating to the repository and its immediate environment (the near field), radionuclide transport through the surrounding rocks (the geosphere), the biosphere, and gas generation and migration. This report describes the biosphere component of that Programme. Additionally DSAT and Site Characterisation work is discussed in so far as is necessary to provide an appropriate context for the NSARP work. It is noted that biosphere studies related directly to the work of the DSAT are described elsewhere [1].

In the title of this report a date of 1994 is adopted to indicate that progress to that date is described. Thus, although the report has been subject to review since that date, it has not been updated to reflect subsequent technical progress in the NSARP.

The general scope of the biosphere research programme and its overall objectives have been described in two previous Current Status reports [2, 3] and in a Reference Document [4], which was structured so as to provide, in convenient form, data of direct relevance to post-closure radiological performance assessments of the proposed facility. This report provides an update on developments in the NSARP biosphere sector over the period subsequent to finalisation of the technical content of the Reference Document [4] in January 1992. In particular, the Reference Document identified several outstanding issues relating to the biosphere and progress in relation to those issues is addressed herein.

1.1 The Biosphere Research Programme

The general scope of the biosphere research programme and its overall objectives remain as described previously [2, 3, 4]. The programme comprises an integrated set of projects relating to climatology, geomorphology, near-surface hydrology and radionuclide transport in soils. In the past, these projects have been complemented by various review studies on the behaviour of specific elements in the environment and o)f particular environmental processes o)f potential significance. Although such review studies are not currently a component of the programme, it is likely that they will he reintroduced within the next two) to three years to ensure that proper account is taken of research developments worldwide that have occurred since the last round of review studies was completed.

The need for a biosphere research programme to support post-closure radiological performance assessments arises because of two considerations:

- The long timescales of relevance for quantitative risk estimation (up to ~ one million years, as discussed elsewhere [1]);
- The specific routes by which radionuclides enter the biosphere.

On the long timescales of relevance to a post-closure radiological performance assessment, climate change is of primary importance in defining the degree of modification of local and regional landforms that is likely to occur and the range of ecosystems that may develop. On the basis of results from the climatic studies, the geomorphological investigations define processes and rates of landform evolution. Separately, these studies also consider the probability of occurrence and magnitude of potential effects on landform of neotectonic (including glacio-hydro-isostatic) movements. Climate and landform, together with postulated vegetational characteristics, provide a basis for evaluating the time-dependent near-surface hydrology of the Sellafield area, which, in turn, provides an input to detailed and assessment level modelling of the distribution and transport of radionuclides in the environment following their release from the geosphere. Such modelling also requires element-specific data and information on a wide range of environmental processes, as provided from the various review studies that have been undertaken.

It is emphasised that biosphere characteristics are of relevance to the post-closure radiological performance of a deep repository because, over very long timescales, small quantities of weakly sorbed, long-lived radionuclides are expected to be released from the near field of the repository, transported through the geosphere and emerge in very low concentrations into the accessible environment. Biosphere processes may then dilute such radionuclides to even lower concentrations, and, indeed, dilution and dispersion in the biosphere play an important part in ensuring that potential post-closure radiological impacts of a repository are very small. For this reason, the biosphere programme includes a substantial component of near-surface hydrological modelling at the catchment scale, with emphasis being placed on the routing of radionuclides through a catchment which they enter via upwelling groundwaters.

Of course, radionuclides are not only diluted and dispersed in the biosphere, they can also be reconcentrated by a variety of physical, chemical and biological processes. In particular, sorption to soils and uptake by plants can play a major role, so these factors are being investigated in a variety of laboratory, lysimeter and field plot experiments, complemented by detailed modelling studies.

When the current status of NSARP biosphere research was last reviewed [4], a number of issues were identified as requiring further work to ensure that the treatment of important processes in the performance assessment models used by the DSAT is robust and adequate for the long-term predictions for which they are being used. These issues were considered to fall into three categories:

- Issues where we are confident that the representations used in assessment models are well founded, but further work is required to obtain refined parameter values;
- Issues that are already treated in assessments, but further work is needed either to underpin the current approach or to develop further representations at an appropriate level for use in assessment models;
- Issues that are not treated explicitly in the current assessment models, and either the

omission needs further justification or a suitable approach needs to be developed that could be included explicitly in the assessment models.

Issues in the first category are largely addressed through on-going programmes of experiment and site characterisation. Here, the issues are mainly of refinement and reducing the uncertainties associated with assessment calculations. Issues in the second and third categories raise larger questions, which often require a number of years of research to address adequately. It is issues in these categories that were highlighted in the previous review [4]. These various issues and their status at January 1992 are briefly summarised below.

With respect to climate and climate change, it was considered possible to sketch out various potential patterns of future climate change to use as input to assessment studies. However; it was also noted that lack of an agreed international policy on limiting greenhouse-gas emissions, limitations in the performance of General Circulation Models (GCMs), lack of knowledge concerning the global carbon cycle, and potential effects of greenhouse warming on ocean circulation patterns and/or cryosphere boundary conditions, meant that it was not possible to provide scientifically based predictions of future climatic conditions at a global and, more particularly, at a regional scale. It was also noted that, for assessment purposes, the climate system, which is continuously variable both spatially and temporally, had been represented as a limited number of climate states. At that time, this approach was considered to be the most reasonable one to adopt, but the view was also taken that, in view of the rapid research developments in climatology, this matter should be kept under review.

In respect of geomorphology, attention was drawn to the considerable debate that had occurred concerning the post-glacial history of the Irish Sea basin. This led to the view that proposed patterns of landform evolution prior to, and, more particularly, subsequent to, any future glaciation must be considered highly speculative. Attention was directed to on-going site characterisation work in the Sellafield area that might help to resolve some of the issues arising. However, it was also noted that limitations in modelling ice sheet development, even given defined future climate scenarios, made it difficult to assess the likely extent and thickness of future British ice sheets.

On the topic of dilution and dispersion, the main issue was identified as being the need to represent the dynamics of processes operating in a spatially heterogeneous domain. Although the research code SHETRAN-UK was already being used to explore this issue, it was emphasised that further research was required. This research was specified to include validation studies for the sediment transport and migration components of SHETRAN-UK, enhancement of the approach to modelling flow in complex lithological sequences and changes to the model to allow longer periods to be simulated.

Finally, it was noted that the experimental lysimeter studies included in the programme had raised some issues relating to the efficiency of uptake of radionuclides by plants from contaminated groundwaters, and that these issues required further investigation.

1.2 Relationship to Assessments and to Characterisation

The biosphere component of a post-closure radiological performance assessment has to take account of results from groundwater modelling on the location and timing of discharges of radionuclides to the biosphere, which is taken to include the superficial Quaternary sediments. It also has to take account of changing characteristics of the biosphere on the long timescales of interest.

To date, the groundwater modelling used to underpin assessments has mainly involved equilibrium studies with time-invariant boundary conditions. However; it is recognised that transient studies may also be required and progress has been made in characterising appropriate calculations.

In this context, the biosphere component of the NSARP has two major roles:

- To define the time-dependent boundary conditions appropriate to groundwater flow and radionuclide transport calculations;
- To specify the environment into which radionuclide fluxes from the geosphere emerge.

Over the timescale of relevance for quantitative or semi-quantitative assessments (one million years), climate and climate change are seen as the primary factors influencing environmental and hydrogeological evolution, though tectonic processes are not neglected. Thus, the NSARP and DSAT programmes have been structured to give priority to studies of climate, land-form evolution and nearsurface hydrology, as well as the potential vegetational characteristics and community structures which could be appropriate to the Sellafield area [1].

Any account of the potential future evolution of the West Cumbrian landscape should be based, in part, on a good understanding of the origin and characteristics of the present landscape. This understanding derives from several closely interacting components of the Nirex programme. Thus, the Site Characterisation programme provides detailed information on the structure of the Quaternary sediments both onshore and offshore, and on the near-surface hydrogeological regime. This information is complemented by DSAT reviews on topics such as soil types, vegetational characteristics, agricultural practices and community structures [1], while NSARP studies emphasise the importance of interpreting the present landscape in terms of past episodes, such as glaciation.

Overall, the aim of the NSARP and DSAT programmes is to establish a comprehensive, self-consistent approach, involving both detailed and assessment type models, that is capable of generating self-consistent futures for the Sellafield area. As discussed below and elsewhere [1], this involves climate modelling to provide a basis for simulations of geomorphological evolution (including ice-sheet, erosion/deposition, sea level and glacio-hydro-isostatic modelling). These geomorphological simulations, in turn, provide a context for near-surface and deep hydrogeological modelling, and for studies of radionuclide distribution and transport in the accessible environment. Of course, the hydrogeological and transport modelling studies also require inputs from the climate modelling, though at a local rather than a regional scale.

1 .3 Structure of the Report

Following this Introduction, Sections 2 to 5 provide detailed accounts of developments in each of the major topic areas within the biosphere component of the NSARP. Thus, climatology, landform evolution, near-surface hydrogeological and contaminant transport modelling, and radionuclide transport in soils and uptake by plants, are addressed separately. In each case, a similar format is adopted. A brief review is given of the status of the research in January 1992, to provide an introduction to one or more subsections describing developments since that time. This then provides a basis for summarising the current status of the research, likely future developments, and its on-going relationship to assessments and site characterisation.

Following these sections on the individual major topic areas, Section 6 outlines the ways in which the NSARP projects relate to other national and international research programmes. In particular; this Section emphasises the close relationships that exist with research programmes concerned with particular aspects of climatology and hydrogeology in contexts other than radioactive waste disposal. These relationships are seen as particularly important in ensuring that the full range of relevant scientific knowledge is made available to Nirex for use in post-closure radiological performance assessments.

Finally, Section 7 summarises overall progress since January 1992, giving particular emphasis to the degree to which previously unresolved issues have been addressed, as well as to the remaining unresolved issues and the work in place to resolve them. Also included is an overall conceptual model of the links between the various factors governing how the biosphere is likely to evolve in the Sellafield area over the next one million years, to provide a context for assessment studies, which are described in detail elsewhere [1].

Within the main text, boxes are used to give supplementary information on specific topics and to present details of research results.

2 Climatology

2.1 Status of the Research in 1992

Because of concerns over global warming caused by enhanced atmospheric concentrations of greenhouse gases, extensive and rapidly developing research initiatives on climate and climate change have emerged worldwide. These initiatives include work on climate change over the whole of the Quaternary, since the dramatic fluctuations in climate over each glacial/interglacial cycle provide many clues as to the processes controlling the climate system. They also include modelling studies using General Circulation Models (GCMs to reconstruct palaeoclimates and evaluate likely global, hemispheric and regional changes in climate due to greenhouse-gas induced warming. In addition, there are longer-term modelling studies which attempt to evaluate how global and regional climates are likely to change on timescales of up to one million years After Present (AP).

In view of this extensive and relevant research effort, it was agreed, when the NSARP climate project was initiated in 1987, that it would he appropriate to limit the scope of the work to review and interpretation of the developing world literature in the context of the particular interests of Nirex. This led to the production of two major review reports [5, 6], which were subsequently utilised to produce a reference text on the nature and causes of climate change [7].

On the basis of these initial studies, it was decided that, for assessment modelling purposes, it is appropriate to represent climatic evolution as a series of discrete states. Spatial and temporal variation within each state was then taken into account in the detailed characterisation of each such state for a particular site [6].

In deriving likely future successions of climate states, the reviews considered the various

1 THE MILANKOVITCH THEORY OF ORBITAL CHANGES

According to the Milankovitch Theory, the Quaternary glacial/interglacial cycles are caused by periodic changes in the seasonal and latitudinal distribution of incoming solar radiation, resulting from variations in three elements of the Earth's orbital geometry.

- Obliquity or tilt: the angle of tilt of the Earth on its rotational axis varies over a 41ka cycle. The effect is greatest at high latitudes and is equal in both hemispheres.
- Precession of the equinoxes: the axis of rotation wobbles due to the gravitational pull of the Sun and Moon on the equatorial bulge and the Earth's orbit is eccentric. The net result of these two factors is that the season at which the shortest Earth-Sun distance occurs varies over 19ka and 23ka cycles. The effects are greatest at low latitudes and opposite in the Northern and Southern Hemispheres.
- Eccentricity: the Earth's orbit varies from near circular to a maximum ellipse with an average periodicity of 95ka. Eccentricity modifies the amplitude of the precessional cycle.

The orbital changes and the accompanying changes in the seasonal and latitudinal distribution of incoming radiation are predictable. Milankovitch argued that glaciation is likely to occur when summer radiation is low (reducing snow and ice melt) and winter radiation is high (providing more evaporation and moisture for snowfall), and that the direct radiation effects are magnified by factors such as icealbedo feedback. This hypothesis could not be tested until the late 1970s when reliable orbital calculations and appropriate geological records*(see Box 2)* became available. The identification of peaks at the Milankovitch frequencies in spectral analyses of global ice volume records extracted from deep ocean cores provided some of the earliest and most convincing support for the Milankovitch Theory*(Figure A).* The dominance of the 100ka cycle was, however, unexpected: prior to this discovery, eccentricity was thought to be important only as a modulator of precessional effects.

1

The phases of the orbital insolation records and ocean core records show good agreement*(Figure B).* Low summer radiation is associated with high global ice volume and vice versa. The ice volume record lags the insolation record reflecting the response time of the major ice sheets to orbital forcing. Evidence in support of the Milankovitch Theory has been extracted from many sources: ocean sediment, landbased sediment, pollen core, ice core, and coral reef sea level records. The secondary orbital periodicities (combinational tones) have been identified in these records as well as the major periodicities.

Results from climate models support orbital forcing as a highly plausible cause of glacial/interglacial cycles, but imply that internal processes and feedbacks play an important part in determining the response of the climate system to the initial forcing. The most plausible internal processes linking the initial Milankovitch forcing to glacial/interglacial cycles are changes in the atmospheric concentrations of $C0_2$ and CH_4, changes in the loading of terrestrial and marine aerosols, ice-albedo feedbacks, and changes in ocean circulation.

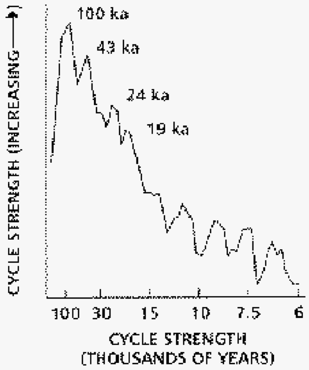

Figure A: Spectral analysis of a 500ka record from two Indian Ocean cores. Peaks of high relative variance are labelled. Data from JD Hays, J Imbrie and NJ Shackleton. Science 194,1121-1132; 1976. Figure from J Imbrie and IZ Imbrie. Ice Ages, Solving the Mystery (Macmillan, London, 1979).

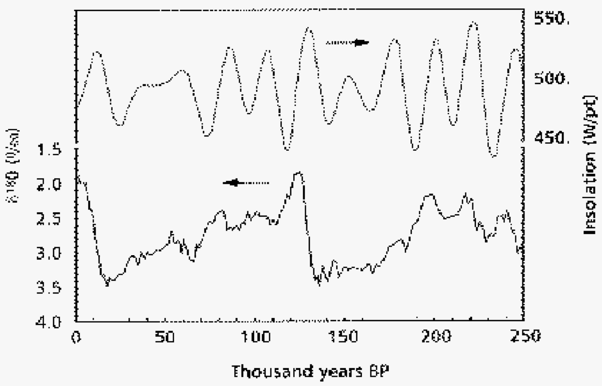

Figure B: Insolation for July at 65ºN (A Berger. J Atmos. Sci., 35, 2362-2367, 1978) and the oxygen isotope record for core RC1 1-120 for the Southern Indian Ocean (JD Hays, J Imbrie and NJ Shackleton, Science, 194,1121-1132,1976). Data from the SPECMAP archives, World Data Center A, Boulder, Colorado.

mechanisms which force climate change and concluded that, over the next one million years, the two that are likely to dominate are changes in the characteristics of the orbit of the Earth, as described originally by Milankovitch (*see Box 1*) and greenhouse-gas effects. It was noted that relationships between orbital forcing and climate change have been studied using a variety of climate models, which have typically been calibrated against, or compared with, the various continuous palaeoindicator records of past climate (*see Box 2*). Several of these models have also been used to project future climates at a global scale.

Although all these models have recognised shortcomings and there are some discrepancies between the future sequences of climate predicted using them, overall they arc considered to provide a reasonably realistic guide to the range of future climate states that would he induced by change in the orbital parameters, if the effects of anthropogenic greenhouse-gas induced warming can he neglected. Specifically, in the absence of an

2 PALAEOCLIMATE INDICATORS

Ocean Cores

The stratigraphic framework for the Quaternary period is provided by deep ocean cores. These records also provide compelling evidence in support of the Milankovitch Theory (Box 1). The most commonly-studied feature of deep ocean cores is their oxygen isotope content, taken to be an indicator of global ice volume. During glacial periods, the oceans are relatively enriched in $^{18}0$, while $^{16}0$-enriched precipitation is trapped in the ice sheets. High $^{18}0$ to $^{16}0$ ratios in seawater therefore indicate a relatively high global ice volume. Past isotope ratios can be estimated from the oxygen isotope content of calcareous marine fauna deposited on the ocean floor. The deposition process is dependent, in part, on temperature and other factors, but about two-thirds of the variance in the isotope-ratio records from calcareous sediments can be related to changes in global ice volume *(Figure A).* Ocean cores are conventionally divided into warm stages (odd numbers) and cold stages (even numbers). According to this convention, Stage 1 is the Holocene, Stage 2 the Devensian glacial maximum, and Substage 5e the Ipswichian interglacial at about 130,000 years Before Present (BP).

Absolute dating is based on the identification of magnetic reversal events in the longest cores, such as the Brunhes-Matuyama boundary (recently re-dated from 730 ka BP to 780 ka BP). Relative dating techniques are used to build up a chronology from these fixed points. This may involve making assumptions about the sedimentation rate and/or tuning the record to the orbital periodicities.

Ocean cores have three major advantages as palaeoclimate indicators. First, they provide long and continuous records. Second they tend to provide a fairly consistent picture of globally synchronous changes. Cores from different parts of the world can be cross-correlated or combined with relative ease. For example, the SPECMAP record which is widely used as the ‘standard’ Quaternary stratigraphy, is a composite of five cores from the Atlantic, Indian and Pacific Oceans. Finally, core samples can be dated reasonably accurately through a combination of absolute and relative dating techniques.

Ice Cores

Ice cores from Antarctica and Greenland provide continuous records from the continents. The records are not as long as those from ocean cores (the longest ice cores extend back to about 250 ka BP whereas some ocean cores extend back to at least 2.5 Ma BP), but generally have a higher temporal resolution (up to the decadal or even annual scale in some cases). The upper sections of ice cores, to about 1 5 ka BP, can be dated by counting the annual layers. Below that, cores are dated using ice flow models and stratigraphic markers such as volcanic dust layers.

Climate records can be reconstructed from ice cores using a variety of indicators, including stable isotope ratios and greenhouse gas concentrations in air bubbles. The oxygen isotope composition of ice cores, for example, is a well established climate indicator *(Figure B).* It depends on air temperature and is also linked to atmospheric circulation changes.

The atmospheric concentrations of $C0_2$ and CH_4 can be reconstructed by measuring the composition of ancient air bubbles trapped in ice cores. The ice core timescale must, however, be adjusted because the ice surrounding each bubble is older than the air trapped within it. The $C0_2$ record from the Vostok ice core *(Figure C)* supports the role of $C0_2$ changes as a positive feedback mechanism in the response of the climate system to orbital forcing *(see Box 1)* and has been used as an input to model-based studies of the last glacial/interglacial cycle (see Box 6).

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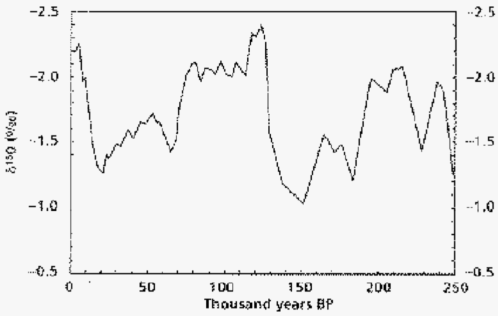


Figure A: Oxygen isotope record of the last 250 ka from core V28-238 in the Equatorial Pacific (NJ Shackleton and ND Opdyke, Quat. Res., 3, 39-55, 1973). Data from the World Data Center A, Boulder, Colorado.

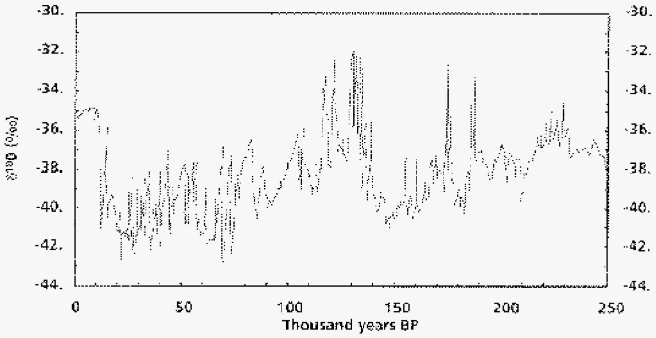


Figure B: Oxygen isotope record of the last 250 ka from the Greenland Ice Core Project (Dansgaard *et al*., Nature, 364, 218-220, 1993; Taylor *et al*., Nature, 361, 432-436 1993). Data from the World Data Center A, Boulder, Colorado.

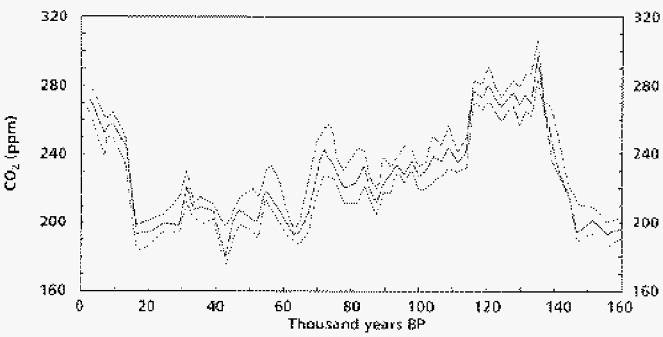


Figure C: Atmospheric concentration of C0 2 reconstructed from the Vostok ice core for the last glacial/interglacial cycle (Barnola *et al*., Nature, 329, 408-414, 1987). Data from the World Data Center A, Boulder, Colorado.

enhanced anthropogenic greenhouse-gas effect, the world's climate should he just beginning a slow deterioration towards glacial conditions. Oscillatory cooling is expected to continue, with progressively colder episodes at 5.0 10^3, 2.3 10^4 and 6.0 10^4 years AP. This last extreme, at 6.0 10^4 years AP, is expected to rival the intensity of the Last Glacial Maximum (which occurred during the Late Devensian, about 18000 years ago) and should be followed by a gradual shift towards warmer conditions.

The models all indicate that climates as warm as the present day have been, and will continue to be, relatively rare. Specifically, the world is not expected to return to conditions matching the Holocene thermal optimum until about 1.2 10^5 years AP.

At the time of the last review [4], preliminary results from a new physically based climate model [8] were available. These preliminary results confirmed that, in the absence of an enhanced greenhouse gas effect, a glacial maximum can be expected in the Northern Hemisphere between 5.5 10^4 and 6.0 10^4 years AP. They also showed that the pattern and range of climatic conditions likely to be experienced over the next one million years will he close to those experienced over the last one million years. This implies that it is reasonable to use the reconstructed record of the Quaternary climate as a guide to future conditions.

Also, by the time of the last review, this new model had been used to investigate the potential effects of enhanced greenhouse-gas warming on long-term climate change. In the study undertaken, it was assumed that such warming would result in melting of the Greenland ice sheet, and it was shown, in consequence, that the glaciation at around 6.0 10^4 years AP would he substantially reduced in severity.

It is emphasised that this preliminary study did not specifically investigate the effects of enhanced greenhouse-gas concentrations. Instead, it postulated particular effects and investigated their implications. Current versions of the model can be used to investigate both the medium term (to 1 10^3 years) and long-term (to 1 10^6 years) implications of enhanced greenhouse gas concentrations (*see subsection 2.3 and Box 6*). However, it is more usual to investigate short-term (~ 1 10*2* years) and

3 GENERAL CIRCULATION MODELS

General Circulation Models (GCMs) are complex, three-dimensional computer-based models of the atmospheric circulation which have been developed by climatologists from numerical forecasting models. They solve the fundamental equations that describe the movement of energy and momentum, and the conservation of mass and water vapour. Physical processes, such as cloud formation, and heat and moisture transport within the atmosphere, and between the atmosphere and the surface, are also described. Atmospheric conditions are specified at a number of ‘grid points’ on a regular grid over the Earth's surface, and at several levels in the atmosphere. The fundamental equations are then solved at each grid point, using numerical techniques. Until recently, the standard approach has been to run such models with the “pre-industrial” atmospheric $C0_2$ concentration (the control or $1xCO_2$ run) and then to rerun the model with doubled $C0_2$ (the perturbed or $2xCO_2$ run). Results are recorded once the model reaches equilibrium. These experiments are, therefore, known as equilibrium response runs. Although they do not take into account time-dependent effects, such as the thermal inertia of the oceans or the transient nature of greenhouse gas forcing, they do have the advantage of requiring less computing time than more sophisticated models. One reason for this is that the ocean is highly simplified with no deep water mixing or transport.

3

Advances in computing power are enabling modelling groups to run time-dependent (or transient-response) experiments, in which CO_2 concentrations increase gradually through the perturbed run. Transient-response experiments require a fully coupled atmosphere-ocean GCM. A common scenario for a transient experiment is to increase $C0_2$ by 1% per annum in the perturbed run *(Figure A)*.

Despite the continuing advances in GCM development, a number of problems remain. For example, even in the current generation of "high-resolution" transient models, the grid has a low spatial resolution relative to the scale of processes such as convective precipitation. The UK Meteorological Office transient model (UKTR), for example, has a relatively high-resolution of 2.5° latitude by 3.75° longitude, but still has a simplified geography *(Figure B)*.

Other problems include:

- Poor representation of sub-grid-scale processes
- Lack of relief and unrealistic geography
- Poor representation of feedback processes particularly cloud feedbacks

In consequence, different models can produce contradictory results, particularly at the regional scale, and for parameters such as precipitation and soil moisture.

The ability of a particular GCM to reproduce the details of the present-day climate must be assessed before output can be used for regional scenario development. This ability varies with scale and the parameter being considered. For example, GCMs are generally better at simulating the mean seasonal temperature cycle for a large region than daily temperature at the sub-regional scale. Similarly, on a daily basis, GCMs are better able to simulate free atmospheric variables such as sea level pressure than variables such as precipitation. Climatologists are developing techniques to generate scenarios, at appropriate temporal and spatial scales, for variables of use to impact analyses. It must, however, be stressed that the reliability of all regional scenarios is constrained by the reliability of the underlying GCM results.

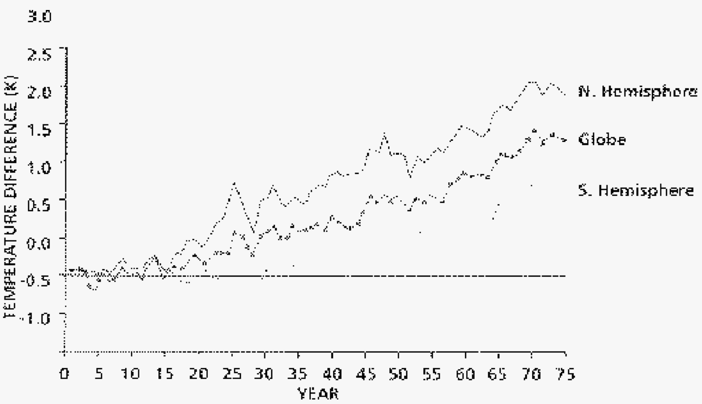


Figure A: Mean change in surface temperature for the globe (solid line), the Northern Hemisphere (dashed line) and the Southern Hemisphere (dotted line) simulated by the UK Meteorological Office high-resolution transient model [UKTR] [(Hadley Centre, Hadley Centre Transient Climate Change Experiment (Meteorological Office, Bracknell, London, 1992)]. CO_2 is increased by 1% per annum over the 75 year-long perturbed run.

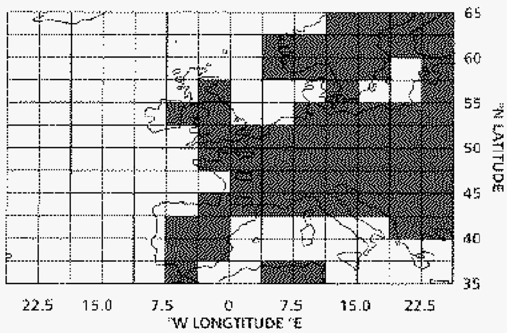


Figure B: grid boxes for the European window of the UKTR model. Shaded areas are land-boxes.

medium term effects of enhanced greenhouse gas concentrations using GCMs (*see Box 3*). At the time of the last review [4], GCMs were mainly being used to model the equilibrium, rather than the transient, response of climate to greenhouse-gas forcing. However, the initial transient results that were available suggested that regional patterns of change differ markedly if transient effects are taken into account. In consequence, it was considered possible that the equilibrium GCM results in which greatest confidence had been placed, such as enhanced high-latitude warming, may be misleading.

By the time of the last review [4], GCMs had also been used to simulate past regional climates. Thus, climate conditions and circulation patterns at selected times in the past had been investigated in snapshot model experiments. Model boundary conditions, including the location and size of ice sheets, and sea-surface temperatures, were prescribed on the basis of palaeoindicator data. Thus, these model experiments had largely been confined to comparatively recent and distinctive episodes, such as the Last Glacial Maximum and Holocene thermal optimum, for which sufficient data were available.

On the basis of these various modelling studies, plus review and interpretation of the palaeoindicator data, it was considered that five broad climate states can be used to characterise the range o)f likely future climatic conditions in Britain: Mediterranean (or Greenhouse), Temperate, Boreal, Periglacial (or Tundra) and Glacial. In order to provide detailed characterisation of each of these states, they were related to a widely used climate classification scheme (a modified version of the one developed by Köppen and Trewartha [9, 10]) and meteorological stations in appropriate geographical regions were selected to provide analogues of the meteorological records that might he characteristic of Sellafield in future climate conditions (*see* [4] *for details of the analogue stations adopted and also Box 5).*

It is emphasised that climate states were characterised using analogue data from meteorological stations to ensure that comprehensive, detailed and self-consistent meteorological data sets would he available as input to hydrological and radionuclide transport models (*see also* [1]). Several analogue stations were selected for each climate state, in order to provide an indication of the degree of variation in climate that might occur within each state.

2.2 Transitions Between Climate States

It was, of course, recognised at the time of the last review [4] that the concept of representing future climate as a sequence of discrete states is a gross simplification. For this reason, a further review study was undertaken to determine whether any important processes or events had been neglected because of the representation of climate change as a succession of discrete stages [11]. Overall, the authors were unable to identify any major features of transition periods which invalidate the treatment of future climate change as a succession of discrete climate states. However, various issues were identified which are being addressed in ongoing research and assessment studies.

- During the period of oscillatory cooling leading to the next glaciation, it is possible that there may occur periods of relatively warm climate, of 1000 to 5000 years duration, that are largely restricted to) the UK and/or northwestern Europe, whilst conditions in other regions remain more severe. Thus, relatively warm conditions in the Sellafield area may occur in conjunction with periods of eustatically reduced sea level.

- If the next glaciation is reduced in extent (because of the effects of enhanced greenhouse warming, for example), then the accompanying isostatic depression will be less. In addition, Sellafield may he close to, or beyond, the UK ice sheet margins and may have a glacial and post-glacial history that is very different from that which occurred during and after the Late Devensian glaciation.
- The changes in coastal topography which will accompany sea level change over the next interglacial-to-glacial transition will have implications for the transport and deposition of sediments at Sellafield. As sea level falls, river channels will cross an increasingly wide plain and sedimentation will occur in an increasingly estuarine environment. Changes in climatic factors, such as the strength and dominant direction of winds, may affect the magnitude and location of both fluvial and aeolian deposition. Overall, there is a need to give further consideration to the processes of sediment movement, deposition and reworking in a transient system. In particular; relationships between the rate of sea level change, changes in coastal topography and changes in fluvial deposition in the offshore environment require investigation.
- Mode changes in the oceanic thermohaline circulation have recently gained popularity as an explanation of the onset and termination of the Younger Dryas cold period about 11,000 years ago. Although there is no convincing evidence that mode changes have occurred during periods of generally cooler/cooling climate, it might be useful to assess the potential implications of a “reversed Younger Dryas-type event”. Such a warming event could occur during a period of glacial-type ocean circulation and might last 1000 to 2000 years. It would he marked by increased North Atlantic Deep Water (NADW) production and by the temporary restoration of the Gulf Stream.
- More generally, whilst it is known that the Gulf Stream is replaced by cold surface currents during glacial periods, it is not possible to predict with any certainty the point in the next (or any subsequent) glacial cycle at which this will occur. For this reason, the implications of shutting down the Gulf Stream at various points in the glacial cycle require consideration.
- Similarly, it is known that a predominantly westerly wind circulation regime dominates during interglacial periods, whereas a more easterly/southerly regime dominates during glacial periods. Again, the point of transition is not known, though it is more likely to occur during a Periglacial than during a Boreal climate. This circulation change has implications for the development o)f future British ice sheets, and for processes of aeolian transport and deposition.
- All other things being constant, enhanced greenhouse warming is expected to cause an expansion of the northern limits, and retreat of the southern limits of individual species of vegetation. Their eventual distribution may be beyond the limits of their range during previous interglacials. The pattern of future vegetation change is, therefore, likely to differ from that of previous post-interglacial periods.
- Once sea level begins to fall, former coastal sediments will be exposed. If the local climate is still relatively mild, or an interstadial-type

warm episode occurs, then these new fertile land areas will provide valuable agricultural resources. The maintenance of seed and genetic data banks may permit the rapid reestablishment of agricultural activity during such episodes.

- More generally, it is not thought appropriate to consider changes in climatic conditions at Sellafield in isolation from changes across the wider northwest European region, since this wider context will strongly condition the impact of the changes occurring at Sellafield.

2.3 Developments in Climate Research

Since January 1992, there has been a variety of developments in climatic research of particular interest to Nirex. Overall, these developments may be characterised under five main headings:

- The implications of new palaeodata on $C0_2$ and CH_4 concentrations in the atmosphere;
- Interpretation of data from new, deep ice cores in Greenland (*see Plate 1*);
- Identification and study of the short-term dynamics of past climate change;
- Studies of a calcite vein from the Devils Hole, Nevada which throws doubt on conventional interpretations of the Milankovitch hypothesis (*see Box 4*);
- Experimental and modelling studies relating to the enhanced greenhouse-gas effect.

These topics are discussed in more detail in the following subsections.

2.3.1 Palaeodata on Greenhouse-gas Concentrations in the Atmosphere

During glacial-interglacial cycles, atmospheric concentrations of the greenhouse gases $C0_2$ and CH_4 are known to vary markedly, being at their lowest during glacial episodes. These changes in concentrations act as a major positive feedback in orbitally induced climate change, which must be taken into account in long-term climate modelling. Conveniently, records of varying $C0_2$ and CH_4 concentrations are preserved in ancient air bubbles trapped in ice cores from Greenland and Antarctica [6].

In the case of $C0_2$, concentrations fell to between 180 and 240 ppmv during the Last Glacial Maximum at about 18000 years Before Present (BP) and rose rapidly, during the period 16,000 years BP to 10,000 years BP, to a concentration of about 280 ppmv (80% of the present value). It was on the basis of this evidence, including the phase relationships between the $C0_2$ record, insolation changes and global ice volume, that it was concluded that the observed changes in $C0_2$ concentrations act as a positive feedback mechanism and not as a driving mechanism of the Quaternary glacial cycles.

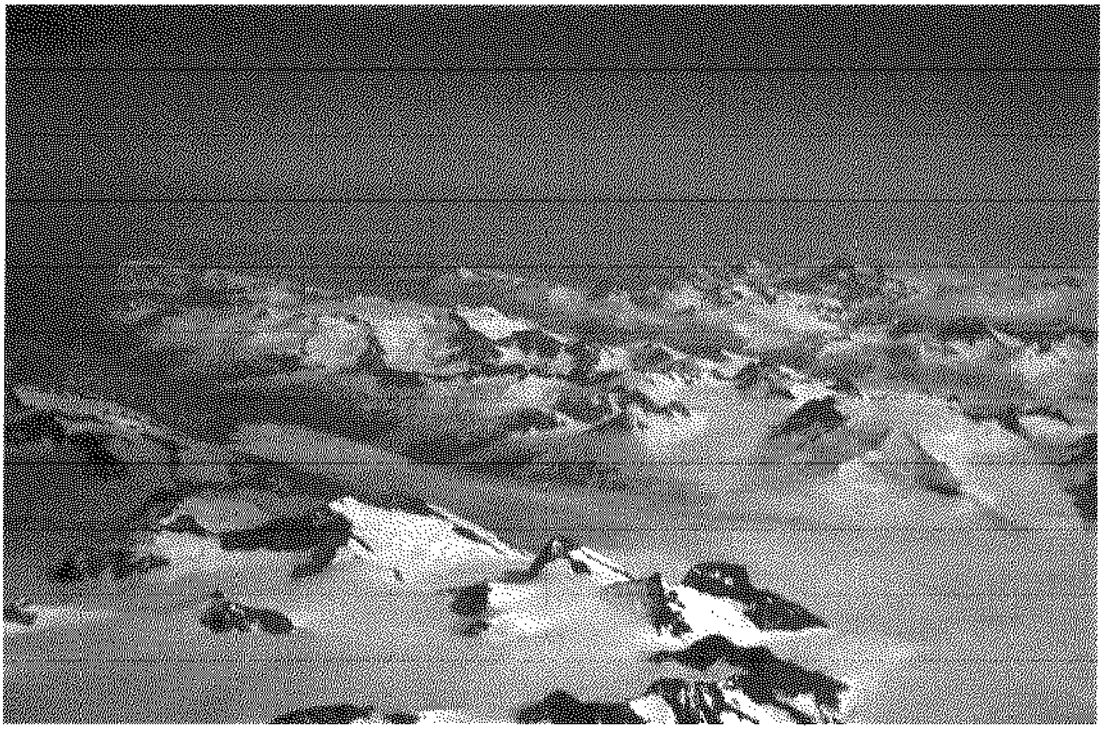
Mechanisms causing changes in atmospheric $C0_2$ concentrations remain obscure. One of the most plausible of those proposed is the biological pump. It is argued that increased high latitude ocean productivity during glacial periods is responsible for enhanced photosynthetic uptake of $C0_2$ in surface waters and the removal, or ‘pumping’, of organic carbon to deeper waters. Shemesh *et al.* [12] have recently tested this hypothesis by analysing organic matter preserved in diatoms from deep sea sediment cores. Their results suggest that primary production in the South Atlantic was lower during the Last Glacial Maximum, rather than higher as required by the biological pump mechanism.

Reversal of the biological pump is just one of many mechanisms which have been proposed to explain the rapid increase in atmospheric $C0_2$ concentrations at the end of the Devensian. This and many of the other hypotheses involve vertical changes in nutrient availability, carbon content and ocean productivity which can be estimated from sedimentary and foraminiferal species data. All these proposed mechanisms should be detectable in sediments because they involve oceanic $\delta^{13}C$ fractionation, as they shift dissolved carbon into deep water, either from the surface or from intermediate waters, to produce a reduction in atmospheric CO_2. Inspection of the data has led Kerr [13] to the view that a biological mechanism involving oceanic $\delta^{13}C$ fractionation cannot explain the variability in atmospheric CO_2 recorded in the Vostok (Antarctica) ice core. He suggests instead a non-biological mechanism which requires less isotopic fractionation. This is based on the observation that dust and sea salt records from Antarctic ice cores indicate that glacial periods are windier than interglacial periods, and thus that the rate of air-sea gas exchange should be higher in glacial than in interglacial periods. In particular, air-sea gas exchanges into poleward-advected, sinking cold water should be increased.

In modelling studies, Kerr [13] has shown that the wind-induced solubility effect outlined above was sufficient to have reduced the atmospheric CO_2 concentration by about 50 ppmv during the Late Devensian glaciation. However, it is only when the wind-induced solubility effect is invoked in combination with a biological pump component that the modelled record of atmospheric CO_2 resembles that observed for the last 150,000 years from the Vostok ice core.

Another potential mechanism which does not

Plate 1 **Greenland ice sheet**



4

THE DEVILS HOLE STUDY AND ITS IMPLICATIONS FOR THE MILANKOVITCH HYPOTHESIS

The 500 ka calcite record from Devils Hole in Nevada is of particular interest because it casts some doubt on the link between Milankovitch cycles and climate change.

The Devils Hole record (Figure A) consists of $\delta^{18}O$ measurements taken from a 36cm core through a calcite vein. It is dated, from 560ka to 60ka BP, by interpolating between 21 replicated mass-spectrometric U-series dates. These are minimum dates only, because they do not take account of the transit time of precipitation from the recharge areas to the point of calcite deposition. It is possible that the true ages are up to 10ka older. The $\delta^{18}O$ 0 content of the Devils Hole record is directly proportional to the temperature of local precipitation. The record is, therefore, interpreted as an indicator of average winter-spring land surface temperature, with the $\delta^{18}O$ values being lower during glacial intervals.

The Devils Hole record shows generally good agreement with the SPECMAP record *(see main text, figure 1)* indicating that the pattern of temperature change in this region mirrors the pattern of global change. There are, however, significant differences in the termination dates taken from the two records. A termination event is the end of a glacial period. It can be defined in any isotope record as the mid-point between a trough, the glacial minimum, and a peak, the interglacial maximum. The authors assign a date of 140 ka BP to Termination II in the Devils Hole record, and find that this event occurred when summer insolation at 60ºN reached a minimum and not, as expected, at an insolation maximum *(Figure B)*. Three out of the four Terminations recorded at Devils Hole are found to precede, or not to be associated with, major peaks in summer insolation. Furthermore, according to the Devils Hole record the average length of interglacial periods is much longer than predicted from Milankovitch-type hypotheses.

Overall, the researchers who have studied the Devils Hole record conclude that "collectively, these observations are inconsistent with the Milankovitch hypothesis for the origin of the Pleistocene glacial cycles but they are consistent with the thesis that these cycles originated from internal non-linear feedbacks within the atmosphere-ice-sheet-ocean system". These conclusions have been criticised, but further research is needed before the Devils Hole controversy can be resolved.

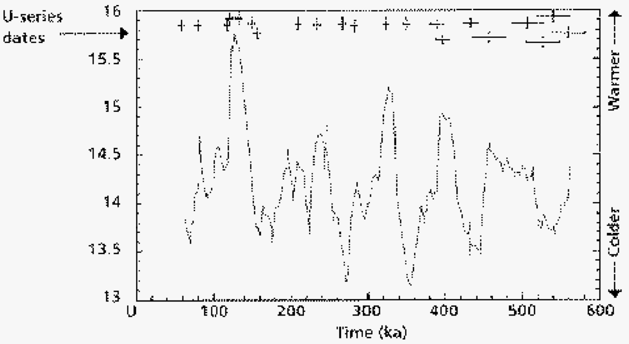


Figure A: The oxygen isotope record from the Devils Hole calcite vein. Mass-spectroscopic U-series dates and their uncertainties are shown above the oxygen isotope record. Figure from IJ Winograd et al., Science, 258 (5080),255-260,1992.

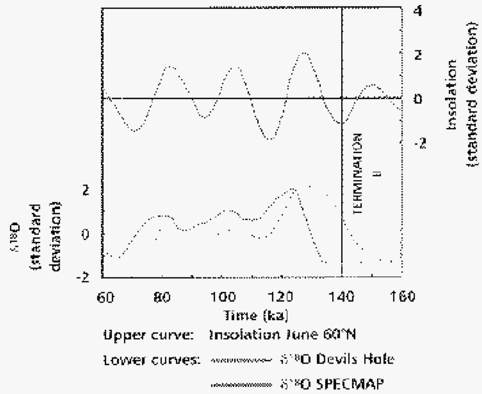


Figure B: Termination 11 in the Devils Hole and SPECMAP records, compared with mid-June insolation at 60ºN. Based on a figure from IJ Winograd et al., Science, 258 (5080),255-260,1992.

require nutrient productivity changes is based on the hypothesis that the rapid increases in atmospheric CO_2 concentrations over a few thousand years at each of the last two glacial-interglacial transitions are related to large releases and subsequent oxidation of subsurface CH_4 [14, 15]. On the basis of a simple model comparing the results obtained with CO_2 concentration data from the Vostok ice core, Loehle [15] concludes that the qualitative fit is remarkable and takes this to indicate that the proposed mechanism gives effects of the right order of magnitude. However, the apparently good fit may simply reflect the fact that similar trends exist in the observed CO_2 and CH_4 records. As the model applies a constant oxidation rate to the CH_4 record, it is inevitable that the model output will be similar to the observed CO_2 record.

Although the contribution of the CH_4 oxidation mechanism to variations in atmospheric CO_2 concentrations is uncertain, CH_4 is also a greenhouse gas in its own right. Recent modelling studies [16, 17] support the view previously advanced [6] that changes in atmospheric CH_4 concentrations are related closely to changes in the extent of wetlands.

Finally, it is noted that extension of the Vostok record back to 200,000 years BP gives further support for the role of CO_2 and CH_4 concentration changes as a positive feedback mechanism in climate change [18]. As a further 1000m of ice remains to be drilled at Vostok, the record from that site could be extended back to around 700,000 years BP. Thus, when this drilling is complete, a very much more extensive dataset will be available to test the various alternative hypothetical mechanisms for how this positive feedback occurs. In the interim, it seems likely that variations in atmospheric CO_2 and CH_4 concentrations will have to be treated as empirical input data in models of long-term climate change (*see subsection 2.4 and Box 6*) .

2.3.2 Data from Greenland Ice Cores

Prior to 1992, studies of climate change based on ice cores from Greenland had suffered from concerns about disturbed stratification and limited resolution. However, in that year, Johnsen *et al.* [19] reported preliminary results from a new deep high-resolution core from central Greenland (*see Plate 1*), which has been drilled under the international Greenland Ice Core Project (GRIP). The site was selected because it was considered to have an ideal depositional environment and iceflow pattern resulting in minimum disturbance of the record. Johnsen *et al.* [19] based their analysis on the first 2300m of the core, which was drilled by summer 1991 and spans the last 40,000 years. Bedrock was finally reached in July 1992, giving a complete core 3028m long covering the period back to 250,000 years BP.

As analysis of the GRIP core has continued, preliminary results have also become available from the US Greenland Ice-sheet Project 2 (GISP2). The GISP2 core was drilled over five years and bedrock was reached on 1 July 1993. The GISP2 site lies 28km west of the GRIP site, sufficiently close for detailed comparisons to be made. This is of particular interest, since both cores provide continuous high-resolution records of climate-related parameters going back at least 200,000 years.

The first comparative study of the two complete cores is provided by Taylor *et al.* [20]. Comparison of electrical conductivity measurements from the two cores reveals that the upper 90% of the records are in good agreement, but that major discrepancies occur in the lower 10% (older than 87,000 years BP). Reasons for the discrepancies in the two records are not yet clear. However, the increasing distortion of dust bands seen in the GISP2 core below 2200m in depth could be associated with ice flow and folding. In this context, it is noted that the GRIP site is located at the present-day ice divide where there is no shear flow to generate ice folds. In contrast, the GISP2 site is considered likely to suffer from shear flow at the present day. However, it is quite possible that, due to climate change, the ice divide has changed position during the period covered by the records. Thus, there is no strong *a priori* reason to consider the GRIP record to be less distorted in its lower part than the GISP2 record [20, 21].

Considering only the more recent part of the records, these new ice-core data reveal that a series of short interstadial (warm) episodes punctuated the Devensian glacial. In addition, during the subsequent warming, short returns to colder conditions occurred on timescales of the order of centuries [20]. More rapid climate change has also been identified. It appears that climate oscillations over time periods as brief as 10 to 20 years occurred during the transitions between longer cold or warm periods. This leads Taylor *et al*. [22] to speculate that the climate system during interstadial events and other transitions acts as ‘a flickering switch’ which fluctuates between two modes before stabilising. Interestingly, a proxy record of sea-surface temperatures for the last 90,000 years [23] seems to confirm the climate instability of the Devensian and indicates that it was not confined to the Greenland area. Nevertheless, it is not yet clear whether the new Greenland ice-core records are measuring anything other than local or regional variability with a magnitude similar to that which occurs today. Once CO_2 records are available from these cores, this matter may be substantially resolved, since CO_2 concentrations are generally considered an indicator of global palaeoclimate.

2.3.3 Short-term Dynamics of Past Climate Change

As outlined in the previous subsection, data from the GRIP and GISP2 ice cores indicate that the majority of the Devensian glacial period was characterised by short-term climate oscillations, with major shifts in ocean and atmospheric circulation having occurred over periods as short as decades. Understanding of the causes and geographical extent of many of these rapid climate events is currently rather limited.

Heinrich events are an important example of short-term variability. They occurred about every 10,000 to 15,000 years from 80,000 years BP to the end of the Devensian, were associated with ice sheet surging leading to large discharges of icebergs from the Laurentide Ice Sheet into the North Atlantic, and each was followed by an abrupt warming [23]. It is speculated that this warming was due to a rapid reduction in the amount of glacial melt water entering the North Atlantic which resulted in a change in the mode of ocean circulation, including restoration of the Gulf Stream. It remains a strong possibility that many of the rapid climate changes within the Devensian which have not been associated with Heinrich events were also related to changes in the strength of the thermohaline circulation and North Atlantic Deep Water production following variations in the flux of melt water entering the North Atlantic.

Short-term variability also occurred during the period of general warming subsequent to the Last Glaciation, which was characterised by a series of abrupt returns to a glacial climate. The best known of these returns is the Younger Dryas. Emerging evidence continues to suggest that this event may have been global in extent. The two new high resolution Greenland ice cores described in subsection 2.3.2 indicate that the Younger Dryas began and terminated in just a few years, and that, within the Younger Dryas, there were frequent, often short (less than 10 year) changes in atmospheric circulation. As with Heinrich events, speculation about the mechanism responsible centres around variations in North Atlantic Deep Water production and the strength of the thermohaline circulation.

One potential process that can induce short-term climate change is periods of high volcanic activity [6]. However, evidence as to whether this is a significant factor remains controversial. Thus, Crowley *et al.* [24] have recently reanalysed the record of acidity levels from the Crete ice core in Greenland, which formed the basis for the classic study by Hammer *et al.* [25] on this topic. Crowley *et al.* [24] demonstrate that the acidity record consists of volcanic-induced spikes super-imposed on a background of acidity of non-volcanic origin. Relatively high levels of background acidity are identified as occurring during the medieval Little Ice Age. Thus, the Little Ice Age acidity peak, which led Hammer et a1. [25] and others to infer a relationship between periods of cold and relatively high volcanic activity, could simply reflect variations in background acidity. Crowley *et al.* [24] link the variations in background acidity with variations in ocean productivity and associated variations in the release of dimethylsulphide to the atmosphere. Changes in acidity could, therefore, be a consequence of climate change rather than an indicator of its cause.

This revised approach leads Crowley *et al.* [24] to suggest that the link between short-term climate variability and volcanic eruptions 1S weaker than previously thought. However, this conclusion is not supported by GCM studies using the Goddard Institute for Space Studies Climate Model II to simulate the response of the present-day climate system to a spatially and temporally constant forcing with volcanic aerosols [26]. Nor is it supported by a detailed study of Northern Hemisphere winter surface air temperature patterns after each of the twelve largest volcanic eruptions which have occurred since l883 [27]. Overall, while volcanic forcing remains a plausible factor in short-term climate change, there continues to he a need for an improved understanding of the mechanism and magnitude of the climatic response to such forcing.

2.3.4 The Devils Hole Controversy

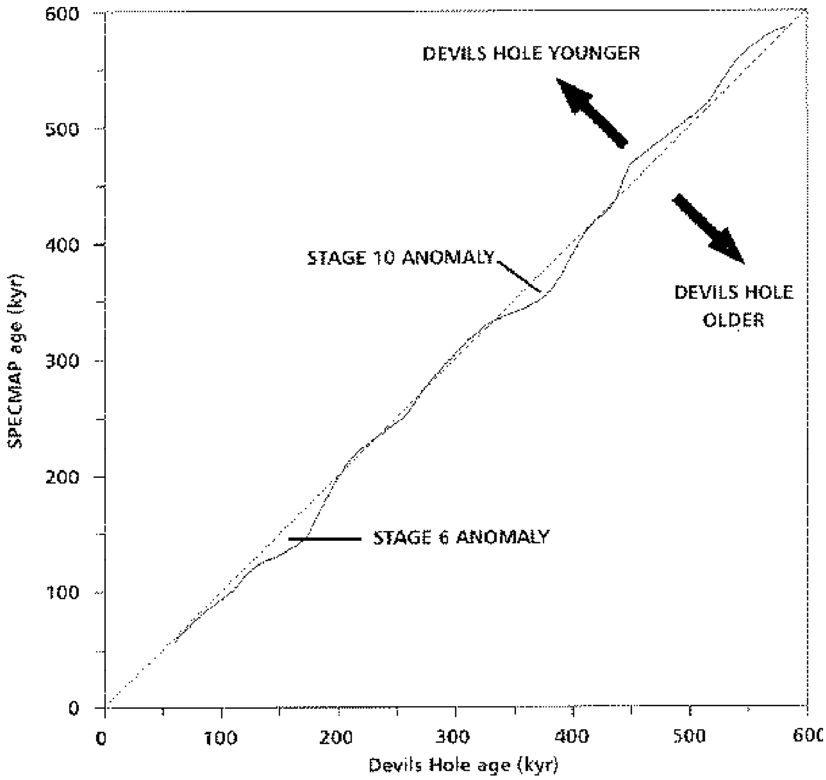
Although the Milankovitch hypothesis of long-term climate change driven by variations in the orbital motion of the Earth is widely accepted by climatologists and provides a basis for modelling long-term future climate changes (*see subsection 2.4*), it has not gone unchallenged. Specifically, in 1988, a 250,000 year climate record based on a Great Basin calcite vein was published [28] and subsequently, in 1992, a new study of a 500,000 year calcite record from the Devils Hole Nevada [29] addressed many of the criticisms of the earlier study. Details of the Devils Hole record and its interpretation are given in box 4.

Overall, the 500,000 year Devils Hole record shows generally good agreement with the SPECMAP ocean core record (*Figure 1*), which leads Winograd *et al.* [29] to conclude that it provides an appropriate palaeoindicator of global climate change. There are, however, some significant differences between the SPECMAP record and the Devils Hole record. Whereas glacial terminations in the SPECMAP record are associated with insolation maxima, three out of four of the glacial terminations identified in the Devils Hole record either precede or were not associated with major peaks in summer insolation. For this reason, Winograd *et al.* [29] conclude that the Quaternary chronology, which is closely tied to the SPECMAP record, requires revision and that their observations are inconsistent with the Milankovitch hypothesis for the origin of the Pleistocene glacial cycles. This view has been challenged by questioning the validity of the $^{234}U/^{230}Th$ dating of the calcite [30, 31], but these challenges do not stand up well to close inspection [32, 33] and Imbrie *et al.* [34] dismiss the hypothesis that the dating of the Devils Hole core is incorrect. They do, however, test the hypothesis that the SPECMAP chronology is incorrect. This is done by tuning the Devils Hole chronology to $\delta^{13}O$ records from four independent ocean cores in widely separated locations, away from continental margins and with very different sedimentation rates. The result of this tuning is that unlikely increases in sedimentation rates are required during glacial maxima at the ocean core sites. In contrast, the original SPECMAP age model produces much more realistic sedimentation rates during these glacial maxima.

Overall, Imbrie *et al.* [34] and Emiliani [35] tend to accept the Devils Hole chronology and imply that both it and the SPECMAP chronology are correct, but not synchronous. This leads to a variety of unresolved issues as to what global and regional measures of climate are recorded in the various records. In particular, difficulties arise as to the duration of the Ipswichian/Eemian interglacial at around 130,000 years BP. This interglacial is estimated to be 11,000 years long in the SPECMAP record, 17,000 years long in the Vostok record [18] and about 20,000 years long in the Devils Hole record [29].

Currently the status and interpretation of the Devils Hole record remains controversial, with many of the criticisms and responses having been published only as correspondence and, therefore, without the benefit of peer review. More generally, a very solid basis of evidence would be required

Figure 1 **The relationship between the SPECMAP and Devils Hole records. From J Imbrie et al., Nature, 363 (6429), 531-533, 1993.**



before it was appropriate to redate events in the Quaternary, because the numerous correlations between the marine record and orbital change are too good to dismiss [36] (*but see also subsection 2.4*). Even if Winograd et a1. [29] are proved correct and the Quaternary chronology does require revision, reconstructions of the range of climate variability experienced during glacial and interglacial periods will remain unaffected and the Quaternary will continue to provide a useful guide to future climate conditions at Sellafield.

2.3.5 Experiments and Modelling Relating to the Enhanced Greenhouse Gas Effect

Much of the discussion of the anthropogenically enhanced greenhouse effect in previous reports [6, 7] was based on the findings contained in the first report from the Intergovernmental Panel on Climate Change, referred to here as IPCC 90 [37]. The IPCC has subsequently reassessed net greenhouse gas emissions and produced a new set of scenarios published in an update to IPCC 90 (IPCC 92 [38]). According to IPCC 92, the new findings “do not affect our fundamental understanding of the science of the greenhouse effect and either confirm or do not justify alteration of the major conclusions of the first IPCC assessment” .

IPCC 92 presented six new scenarios based on different assumptions about population and economic growth, technological development, resource limitations, fuel mixes, agricultural development and implementation or not of remedial policies which have already been proposed. All six of these scenarios are considered as replacements for the single IPCC 90 Business As Usual scenario. However, none of the new IPCC scenarios includes the negative forcing from sulphate aerosols or stratospheric ozone depletion.

Wigley and Raper [39] have included some of the factors omitted by the lPCC in revised versions of the lPCC 92 scenarios. Their best estimates of global warming from 1990 to 2100 for all six new scenarios range from 1.5ºC to 3ºC, when negative feedbacks are included.

Although the scientific consensus is that global warming projections need to be revised downwards, in part because of the existence of negative feedbacks, the extent to which these newly recognised mechanisms may offset or even cancel out the impact of the greenhouse gases remains controversial. The sulphate feedback mechanism has caused particular controversy, and it is becoming clear that the overall climate effects of sulphate aerosols, as well as regional distinctions in their impact, are governed by a variety of factors [40]. Sulphate aerosols cause surface cooling by two mechanisms [40]. First, they directly scatter short-wave solar radiation. Secondly, they indirectly affect the short-wave reflective properties of clouds and cause an increase in planetary albedo. However, sulphate aerosols are short-lived, so the time and location of emissions must be considered.

The main source of sulphate aerosols over land is the combustion of fossil fuels. Over the oceans, dimethylsulphide emissions are the most important source. These sulphate aerosols cause increases in cloud albedo through two mechanisms, reduction in cloud droplet size and increased liquid content of the cloud. Kim and Cess [41] have used satellite data to demonstrate that cloud albedos are higher near eastern coastal boundaries in the Northern Hemisphere, as would be expected if sulphate aerosol effects were significant. In contrast, at the global scale, Engardt and Rodhe [42] have been unable to demonstrate from the instrumental record that sulphate aerosols have caused any significant cooling over the last hundred years.

Modelling studies on the expected degree of sulphate aerosol forcing [40, 43] give results that vary by a factor of about two, but agree that a significant negative feedback effect is to be anticipated.

Evaluation of the likely significance of enhanced greenhouse gas concentrations in the longer-term is made more difficult because of ongoing limitations in knowledge concerning the global carbon cycle. It has been shown that there is a discrepancy of some 3 to 4 10^9 tons per year between known CO_2 emissions and the observed atmospheric concentration of CO_2. This discrepancy is still unresolved, though recent evidence supports the terrestrial biosphere as the missing carbon sink [44, 45, 46, 47]. Another unresolved problem is how to account for the decrease in the rate of rise of atmospheric CO2 concentrations since the Mount Pinatubo eruption in the summer of 1991 [48]. It has been speculated that the decrease is a response of the carbon system to the global cooling observed following the eruption. Overall, a better understanding of the global carbon cycle is needed to improve the emissions/ uptake scenarios used in GCMs and to increase confidence in climatic predictions.

At the time of the last major review [6] initial results from transient GCMS were just becoming available. Subsequently, there has been an increase of work in this field. Of particular note is the study by Manabe and Stouffer [49], who used a coupled atmosphere-ocean GCM and a simple model of land surfaces to study the evolution of global climate over the next 500 years. The estimated global surface temperature rise over the next 500 years is 3.2°C, for a doubling of present-day CO_2 concentrations within 70 years, and 7°C for a quadrupling of CO_2 within 140 years. A forcing equivalent to a quadrupling of CO_2 over the next 140 years is a possibility, if present policies to curb greenhouse gas emissions prove inadequate. The Manabe and Stouffer study [49] is particularly useful because it helps to bridge the gap in timescale between simulations performed with conventional GCMs and with the Louvain-la-Neuve model (*see Subsection 2.4*).

2.4 Assessing Patterns of Future Climate for Sellafield

On the basis of work undertaken by the time of the previous review of the NSARP biosphere sector [6], two climate state sequences were developed for the last glacial/interglacial cycle, reflecting two different interpretations of the land-based geological data. These sequences are summarised over (see also [4]).

Two climate sequences for the next glacial/ interglacial cycle were also developed based on orbital climate models. These were designed to represent conditions with and without enhanced greenhouse-gas warming, and are summarised here.

For each climate state, conditions were characterised in detail using the analogue station approach described in subsection 2.1 and Box 5.

Climate Sequences for the Last Glacial/Interglacial Cycle

Index I		Index II	
ka BP	**Climate State**	**ka BP**	**Climate State**
125 - 115	Temperate	125 - 115	Temperate
115-70	Boreal	115 - 83	Boreal
70 - 60	Glacial	83 - 78	Temperate
60 - 55	Boreal	78 - 70	Boreal
55 - 26	Periglacial	70 - 26	Periglacial
26 - 15	Glacial	26 - 15	Glacial
15 - 11	Boreal	15 - 11	Boreal
11 - 10	Periglacial	11 - 10	Periglacial
10 - 9	Boreal	10 - 9	Boreal
9 - 0	Temperate	9 - 0	Temperate

Climate Sequences for the Next Glacial/Interglacial Cycle			
Index I: Without Greenhouse-gas Induced Warming		**Index II: With Greenhouse-gas Induced Warming**	
ka AP	**Climate State**	**ka AP**	**Climate State**
0 - 2	Temperate	0 - 1	Mediterranean
2 - 21	Boreal	1 - 25	Temperate
21 - 25	Periglacial	25 - 50	Boreal
25 - 42	Boreal	50 - 65	Periglacial
42 - 52	Periglacial	65 - 100	Boreal
52 - 62	Glacial	100 - 115	Periglacial
62 - 65	Periglacial	115 - 125	Temperate
65 - 100	Boreal		
100 - 115	Periglacial		
115 - 125	Temperate		

The two indices of future climate relied heavily upon preliminary results from the Louvain-la-Neuve model, in which the long-term effects of greenhouse-gas warming were simulated by assuming that the Greenland ice sheet had melted and assessing the implications of this change in model boundary conditions. In the current programme of research, the Louvain-la-Neuve model is being used more directly to assess future patterns of climate change at Sellafield and this approach is outlined in subsection 2.4.1.

It was also recognised that none of the land-based sequences of palaeoindicator data used in developing the climate sequences or assigning the analogue meteorological stations was based on an Atlantic margin site similar to Sellafield. For this reason, work was put in hand to identify such a site and obtain data from it. Progress in this area is outlined in subsection 2.4.2, which also provides an account of how existing palaeoindicator data are being reassessed in the light of the new ice core data and results from the Devils Hole (*see subsection 2.3*).

2.4.1 Application of the Louvain-la-Neuve Model

The Louvain-la-Neuve model (*see Box 6*) is a sectorised 2.5 dimensional atmosphere-ocean climate model asynchrononsly coupled with an ice sheet model. Version 1 was used in the simulations described above. Since then, Versions 2 and 3 have been developed which include a number of modifications [50, 51, 52]. Despite the improvements associated with these modifications, a number of discrepancies remain between the reconstructed ice volume record [53, 54] and the simulated record. These discepancies are attributed to a number of key processes which are still omitted from the model [52]: changes in atmospheric concentrations of greenhouse gasses and aerosols, cloud variability, sea-level change, changes in deep ocean circulation and changes in water vapour transport.

The deficiencies identified in model Version 3 have been partly remedied by forcing the model with atmospheric CO_2 concentrations derived from

5

CHARACTERISTICS OF THE CLIMATE STATES

Four climate states are used to describe the range of conditions over the British Isles throughout the Quaternary: Temperate, Boreal, Periglacial or Tundra, and Glacial. The effects of enhanced greenhouse warming are represented as an additional state, Mediterranean. The climate characteristics of these states are specified from present-day instrumental analogue data.

Estimates of climate conditions during the past, taken from palaeoclimatic evidence, are used as a guide to the selection of appropriate analogues for the Boreal, Periglacial and Glacial climate states. The palaeoclimatic evidence is applicable to the general region of northern England, but does not provide site-specific information. The effects of changing sea level on altitude continentality and seasonality at Sellafield are, however, taken into consideration in selecting the analogue data. Output from General Circulation Models is used as a guide to the selection of analogue data for the Mediterranean climate state. Appropriate analogue sites are identified using a modified version of the Köppen - Trewartha climate classification scheme. This scheme divides climate into classes according to a set of temperature-based criteria meaningful in terms of the natural vegetation. The selection of analogue data is inevitably somewhat subjective but has been based on some general principles. For example west coast stations are preferred to those from other coasts or from continental interiors, and stations with an altitude of rnore than about 100m are not used.

Climate State	Sellafield Analogue Data
Glacial/extreme periglacial	Jakobshavn, Greenland; Mys Uzlen, Russia; Ostrov Dikson, Russia
Periglacial	Murmansk, Russia; Bethel, Alaska
Boreal	Bodo, Norway; Tromso, Norway; Haparanda, Sweden
Mediterranean	Bordeaux, France*
	La Coruna/Santander, Spain; Tirana/Vlora, Albania; Horta, Azores

(*This analogue station represents a snapshot scenario of the time at which a total transient regional warming of 3oC has been reached, sometime towards the end of the next century or early in the twenty-second century. The other Mediterranean analogues represent progressively more extreme scenarios, greater warming).

Differences between mean annual temperature for Sellafield and the analogue stations are shown in Figure A. Mean annual temperatures across the range of Mediterranean analogue stations show a progressive increase from Bordeaux to Horta.

Similarly, mean annual temperatures show a progressive decrease across the range of cold analogue stations from Bodo to Ostrov Dikson. This suggests that the analogue data are representative of the full temporal variability within each climate state. This helps to overcome some of the possible criticisms relating to the representation of climate as a series of discrete stages.

Whilst it must be accepted that there is no such thing as a perfect analogue, the selection and assessment procedures used in the Nirex climate studies attempt to ensure that the most suitable available sites are employed. The principal advantage of the analogue approach is that the impacts of climate change can be readily assessed from the observed climate records of the analogue stations.

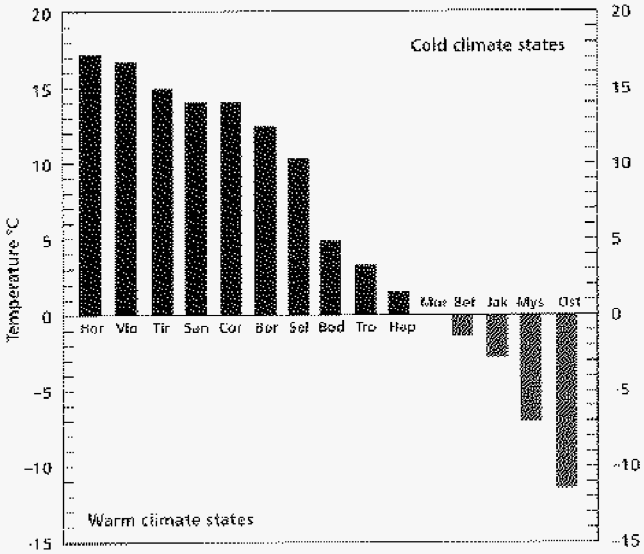


Figure A: Mean annual temperature for Sellafield and the analogue stations.
Hor: Horta, Vlo: Vlora, Tir: Tirana, San: Santander, Cor: La Coruna, Bor: Bordeaux, Sel: Sellafield, Bod: Bodo, Tro: Tromso, Hap: Haparanda, Mur: Murmansk: Bet: Bethel: Jak: Jakobshavn, Mys: Mys Uzlen, Ost: Ostrov Dikson

the Vostok ice core, as well as orbitally related insolation changes. By comparing this run with one without time-dependent CO_2 forcing, Berger *et al*. [55] attribute 50%, of the temperature change and 30% of the ice volume change in the Northern Hemisphere at the Last Glacial Maximum relative to the present day to variations in atmospheric CO_2 concentrations.

In the current research programme, the Louvain-la-Neuve model is being used to provide data relevant to long-term climate change at Sellafield. In addition, more detailed outputs are being provided from a variant of the model to provide data relevant to long-term climate change at Sellafield. In addition, more detailed outputs are being provided from a variant of the model to provide a basis for comparison with the GCM studies that are now being undertaken (*see subsection 2.3.5*).

Specifically, the basic model is being used, with orbital plus greenhouse gas forcing to provide:

6 THE LOUVAIN-LA-NEUVE MODEL OF LONG-TERM CLIMATE CHANGE

To investigate the response of the climate system to orbital forcing, a physically realistic model of the time-dependent behaviour of the coupled climate system is required which must include the atmosphere, oceans, cryosphere, lithosphere and biosphere. Because very long time scales must be modelled a full three-dimensional representation of the Earth-atmosphere system is not feasible with current computing power and speed. Instead, a secorially averaged (essentially two-dimensional) model is under development by A Berger and colleagues at the University of Louvain-la-Neuve, Belgium.

At present, the Northern Hemisphere alone is modelled. The climate model is asynchronously coupled to dynamic models of the Greenland, North American and Eurasian ice sheets. The ocean is represented by a mixed-layer model. The ice-sheet model is updated using a time step of 1ka, with the climate model using a much shorter time step of a few days. There is no geography in the conventional sense. There are seven sectors in each 5º latitudinal band: open ocean, sea ice, ice-free land, snow-covered land, and three continental ice sheets. Over some time intervals of the simulation, some of the continental ice sheet sectors may be ice-free. Internally generated estimates of temperature, sea ice, snow depth and ice-sheet elevation are used as inputs to the next time step, so that the model generates its own boundary conditions. In the palaeoclimate experiments, forcing is provided by daily insolation receipts at each latitudinal band.

The model has been used to simulate the volume of the three major Northern Hemisphere ice sheets over the last interglacial-glacial cycle. The volume of the Antarctic ice sheets is interpolated from volumes at 18ka BP (from palaeoclimate evidence) and today, and combined with the model output to produce an estimate of global ice volume. Results from Version 3 of the model are shown in Figure A. Model performance is assessed by comparison with an oxygen isotope record of global ice volume. The model and reconstructed ice volume records agree reasonably well*(Figure A).* Unlike earlier versions, Version 3 is successful in melting the ice sheets following the Last Glacial Maximum and does not overestimate the present-day ice volume. A number of discrepancies between the reconstructed and model records are, however, evident. For example, the ice volume at the Last Glacial Maximum and the southward extent of the Northern Hemisphere ice sheets are underestimated, and the extent of ice melt over the period 80 - 65ka Before Present (BP) is overestimated by the model.

These discrepancies are attributed to a number of key processes omitted from Version 3: changes in atmospheric concentrations of greenhouse gases and aerosols, cloud variability, sea-level change, changes in deep-ocean circulation and changes in water-vapour transport. A sensitivity study has been performed using a CO_2 record derived from the Vostok ice core *(see Box 2, Figure C)* together with insolation changes as forcing factors.

Model performance is assessed as before using an oxygen isotope ice volume record*(Figure B).* A number of deficiencies identified in Version 3 are partly remedied by the inclusion of CO_2 as a forcing factor. The Last Glacial Maximum ice volume is slightly over-estimated rather than under-estimated. A new error is introduced over the period 63 - 60 ka BP, for which ice volume is severely over-estimated.

The Louvain-la-Neuve model is a valuable tool for investigation of the climate response to orbital forcing and the enhanced greenhouse effect over very long time scales. The model requires further refinement to include important processes, such as deep-ocean circulation, which are currently omitted. Over the next few years, the Louvain-la-Neuve group have plans to incorporate many of these processes into the model.

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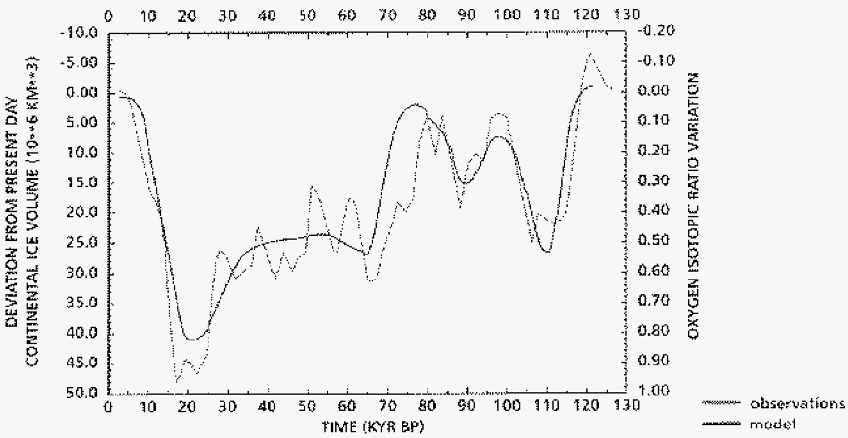


Figure A: Global ice volume simulated by the Louvain-la-Neuve model for the last 122ka (solid line) compared with the reconstructed record. The model is forced by insolation only. The reconstructed record is from LD Labeyrie et al., Nature, 327 (6122), 477-482, 1987 and the figure is based on A Berger et al., Journal of Glaciology, 39 (131), 45-49, 1993.

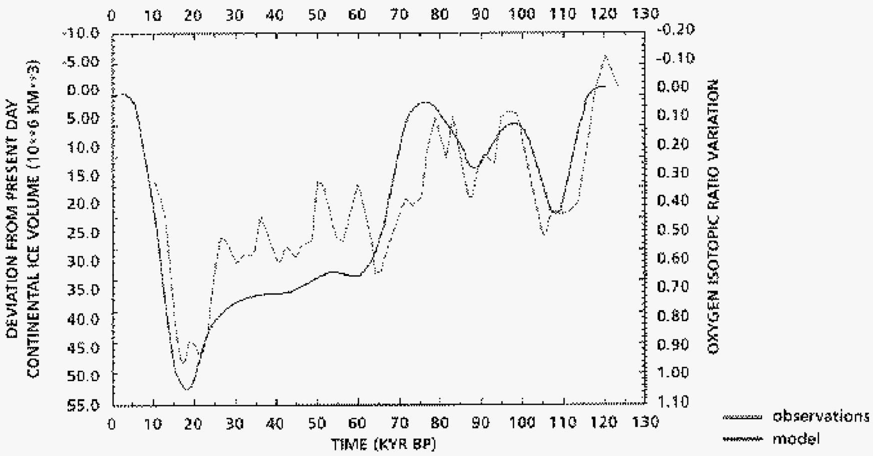


Figure B: Global ice volume simulated by the Louvain-la-Neuve model for the last 122ka (solid line) compared with the reconstructed record. The model is forced by insolation and the Vostok CO_2 record. The reconstructed record is from LD Labeyrie et al, Nature, 327 (6122), 477-482, 1987 and the figure is based on A Berger et al., Journal of Glaciology, 39 (131), 45-49, 1993.

- Global ice volume at intervals of 1,000 years for the next 100,000 years;
- Monthly and annual average temperatures for the various sectors (ocean, sea ice, land surface covered or not by snow or ice) and for the 18 latitude bands between the equator and the North Pole at intervals of 1,000 years for the next 100,000 years.

In separate 100 year simulations, based on the various IPCC scenarios, a new version of the model incorporating the deep oceans is generating, for every month, for different latitude bands:

- Temperature and depth, of the mixed layer for the ice-free ocean;
- Sea ice surface temperature and depth, and the fraction of the ocean covered by ice;
- Surface temperature for the snow-free continent and water availability factor;
- For the continental snow field, the temperature at the top and base of the snow layer, its depth and the fraction of the continent occupied by snow;
- The surface temperature at the top of the ice sheet.

Although the Louvain-la-Neuve model provides some information on regional climate, it operates at too coarse a resolution to provide the detailed information required for hydrological modelling of the Sellafield area. Methods of downscaling results from the model are currently being investigated, concentrating on the key meteorological variables of temperature and precipitation on a seasonal and/ or monthly basis.

The model output available at monthly intervals will be compared, in the first instance, with output from the European window of the UK Meteorological Office high-resolution transient model [56], since these data are already available through a joint Climatic Research Unit/Hadley Centre Link Project [57]. This comparison will not only assist in validating the Louvain-la-Neuve model, it will also provide data relevant to the general downscaling of results from that model.

2.4.2 Generation and Application of Palaeoindicator Data

As described in box 2, a wide variety of palaeoindicators of climate are available and many of the climate records based on these indicators have been taken into account in the completed reviews [5, 6, 7, 1l] However, new long period records continue to arise or are extended in time, while studies such as those undertaken on the Devils Hole calcite vein raise issues which are often best addressed by reconsidering the assumptions that underlie published interpretations of the existing palaeoindicator records.

It is in this context that a variety of palaeoindicatcor data sets have been obtained from the archives held at the National Geophysical Data Center, Boulder, Colorado and, in some cases, from the originators of the data. The most relevent data sets already acquired or being obtained comprise:

- The original oxygen isotope records from deep sea cores used in the SPECMAP analysis [58];
- Newly derived series from deep-sea cores, including $\delta^{18}O$, $\delta^{13}C$, CO_3, Cd/Ca and sea-surface temperature estimates [59];
- CO_2, CH_4, dust and reconstructed temperature series for the last 150,000 years from the Vostok ice core [60, 61, 62];
- Sea-level estimates from coral [63, 64, 65];
- Calculations of orbital parameters for the last 5 10^6 years [66, 67];
- Data from the Devils Hole [29], GRIP [68, 69] and GISP2 [20].

Because many of the published time series are tuned to the orbital record, it makes it difficult to resolve dating controversies, such as that which has arisen in relation to the Devils Hole data. It is, therefore, intended that the original time series from the ocean and ice cores shall be used to re-examine age-depth relationships, to provide a basis for reassessing leads and lags in the response of the climate system to orbital forcing and to investigate a number of specific issues such as the duration of the Ipswichian/Eemian interglacial and the timing of glacial terminations in relation to insolation maxima (*see Box 4*).

As noted above, one of the limitations of the land-based palaeoindicator data is that none of the existing long records relates to a site on the North Atlantic margin. Thus, previous review studies have placed considerable reliance on palaeoclimatic interpretation of pollen records from more continental locations [6,70] However the Laboratory of Historical Botany and Palynology at the University of Marseilles, who have undertaken detailed palaeotemperature and palaeoprecipitation reconstructions at other European sites (*eg* [71, 72]), have identified an important interglacial sediment sequence at Dinge, north of Rennes [73]. Currently, coring of this site is being undertaken as part of the NSARP and the intention is to conduct palynological, palaeobotanical, palaeoentomological and palaeomagnetic studies on these cores with a view to providing quantitative climatic reconstructions back at least as far as the Ipswichian/Eemian interglacial. These reconstructions should then form a major input to work on downscaling from the Louvain-la-Neuve model results to regional climatic characteristics suitable to the oceanic marginal location of Sellafield.

2.5 Status of the Research and its Relationship to Assessments

When the last review of the research programme was undertaken [4], it was noted that lack of an agreed international policy on limiting greenhouse-gas emissions, limitations in the performance of GCMs, lack of knowledge concerning the global carbon cycle and potential effects of enhanced greenhouse warming on ocean circulation patterns and/or cryosphere boundary conditions, meant that it was not possible to provide scientifically based predictions of future climatic conditions at a global and, more particularly, at a regional scale. It was also noted that the simplification, adopted for assessment purposes, of representing climate as a succession of a limited number of different types of climate states would have to be kept under review.

Although it remains true that the future of greenhouse-gas emissions remains uncertain the availability of six alternative IPCC scenarios [38], as enhanced by Wigley and Raper [39*] (see subsection 2.3.5*), means that an internationally accepted basis exists for exploring the climatic implications of a variety of emissions scenarios which incorporate different assumptions about population and economic growth, technological development, resource limitations, fuel mixes, and implementation or not of remedial policies which have already been proposed. In parallel, the capacity of GCMs has been extended and the potential for performing transient model experiments for simulation periods of several hundred years has been demonstrated. Thus, it is now feasible to determine the climatic implications of alternative greenhouse-gas emissions scenarios on timescales more appropriate to the likely persistence of their effects.

Of course, the adequacy of transient GCMs in terms of their ability to capture the important characteristics of the evolving climate system, is at an early stage of exploration. It has already been mentioned that the implications of some mechanisms of climate change, eg the magnitude of negative feedbacks due to sulphate aerosols, remain controversial (*subsection 2.3.5*), while the relationship between emissions and atmospheric concentrations of the greenhouse gasses is uncertain because of limitations in knowledge concerning the global carbon cycle (*subsection 2.3.5*). Nevertheless, over the next two to three years, it should become increasingly possible to make statements concerning the quantitative climatic implications of various greenhouse gas emissions scenarios. This is not only because of the increasing capability of transient GCMs to simulate future climates, but also because the rapidly developing database of palaeoindicator data (*see subsections 2.3 and 2.4.2*) is likely to provide indications of the key factors that should be taken into account. Thus, for example, data on changes in atmospheric CO_2 concentrations since the end of the Devensian may place constraints on the range of possible mechanisms by which carbon is transferred from the atmosphere to the *oceans (subsection 2.3.1*).

Although transient GCMs have the potential to provide quantitative estimates of both global and regional climate change on a timescale of a few hundred years, they cannot be used to establish likely patterns of climate change over the long timescales of interest in post-closure radiological performance assessments. At the time of the last review, projections over the next one million years were made on the basis of results from various semi-empirical models plus first results from the 2.5 dimensional model developed at Louvain-la-Neuve (*see subsection 2.4.1 and Box 6*). Subsequently, development and application of the Louvain-la-Neuve model has been rapid and it is now preferred over the semi-empirical models for making long-term projections of climate at the global scale. Thus, the NSARP climatology programme has moved from a passive review role to having an active role in running this model and interpreting the results obtained (*subsection 2.4.1*). This will facilitate not only the generation of results of direct relevance to post-closure radiological performance assessments, but also comparison of the short to medium term characteristics of the results obtained with output from transient GCM experiments (*subsection 2.4.1*). Such comparisons will be of use in downscaling results from the Louvain-la-Neuve model to a regional or local scale appropriate to Sellafield.

The Louvain-la-Neuve model is driven by processes which force climate change. Currently, the two regarded as of primary importance are orbital forcing and variations in atmospheric greenhouse gas concentrations, though other potential forcings, such as periods of vulcanism, are continually kept under review (*subsection 2.3.3*). Orbital forcing, generally characterised as the Milankovitch hypothesis, has received some criticism in recent years, because of results obtained from the Devils Hole calcite vein (*subsection 2.3.4*). In addition, extensive new data are becoming available from analyses of ice cores (*subsection 2.3.2*), which need to be taken into account in modelling studies, especially as these data include measurements of greenhouse gas concentrations which are used to force the Louvain-la-Neuve model. Thus, there is a need to re-examine all the available palaeoindicator data with a view to determining their self-consistency, and providing input for use with the Louvain-la-Neuve model in simulations of past climates. Appropriate palaeoindicator data will also provide information relevant to downscaling results from the Louvain-la-Neuve model to the Sellafield context (*subsection 2.4.2*).

Currently, it remains the intention to represent climate change in terms of a sequence of a limited number of different types of biosphere states. However, it is recognised that a more continuos representation may be required (*eg* for time-dependent groundwater modelling). Thus, the characteristics of transition climate states have been reviewed (*subsections 2.2*) and literature on the short-term dynamics of climate change continues to be studied in detail (*subsection 2.3.3*). It is emphasised that work with the Louvain-la-Neuve model, which is seen to be central to future developments, will provide time-series of climatic parameters which will have to be interpreted as sequences of climate states. Thus, it will not be difficult to represent climate change as a quasi-continuous process, if this is found to be appropriate.

In summary, it is now considered appropriate to move from a descriptive account of future climate change to an approach which gives greater weight to model simulations. This reflects the rapid developments in climatological modelling which have occurred over the last two years, complemented by the ever-increasing volume and quality of palaeoindicator data, and by the definition of a range of greenhouse-gas emissions scenarios that have a degree of international acceptance and can be used as a basis of assessments. On-going uncertainties relate to the ability of the existing generation of models to capture the important characteristics of the evolving climate system, the ways in which orbital forcing and variations in greenhouse gas concentrations interact to drive climate change, and proper approaches to downscaling model results to a local context. All these aspects are being addressed in the NSARP programme and by the climatological community worldwide.

3 Landform Evolution

3.1 Status of the Research in 1992

At the time of the last review of the NSARP biosphere sector [4] it was stated that work to date had largely concentrated on providing descriptions of the geomorphological processes operating in the range of climatic conditions likely to occur in the British Isles rather than on detailed modelling of the effects of those processes. However it was also indicated that more quantitative studies specifically the modelling of landform evolution would be instituted when this became appropriate.

The descriptive reports that had been completed at the time of the last review related to the Glacial Periglacial and Boreal climate states. However the report on the Glacial state raised some major issues which were addressed in further study. Thus a revised and much expanded version of that report has subsequently been produced [73].

While it is true that the NSARP geomorphological studies through to 1992 had concentrated on providing descriptions of the processes operating in the various future colder climate states identified as appropriate to the British Isles preparatory work had been put in place to develop a digital relief map of Northern Britain with the aim of developing methods of analysis which would permit reconstruction of the palaeorelief of selected areas and in consequence would facilitate the generation of potential future patterns of relief consistent with the climate evolution scenarios adopted. In addition it was recognised that modelling of possible future British ice sheets could be of considerable significance in post-closure radiological performance assessments [75].

Thus, in 1992, it was recognised that future glacial episodes are likely to be of significance in the context of a repository at Sellafield; more work needed to be done to clarify the characteristics of past glaciations in Britain; questions could be raised concerning the adequacy of existing ice sheet models; and that the digital relief map then under development provided a potential tool for exploring some of these issues as well as others relating to neotectonics. In view of the existing unresolved issues it was stated that “the postglacial history of the Irish Sea basin is the subject of considerable controversy and patterns of landform evolution prior to, and more particularly subsequent to any future glaciation must be considered highly speculative” [4]. It was also noted that “a current research program on The nature of the Quaternary sediments, both on and off shore in the Sellafield area is likely to yield a substantially enhanced understanding of events subsequent to the peak of the Last Glaciation on a timescale of one to two years” [4].

The issues re1ating to glaciation set out in 1992 have largely defined the scope of the subsequent NSARP geomorphology programme and have had a significant impact on the Site Characterisation programme at Sellafield. The work that has been undertaken is described in the following subsections. Thus subsection 3.2 outlines the new picture of Glacial Britain that has emerged and sets a context for evaluating its implications for the development of the Cumbrian landscape. This provides a basis for subsection 3.3 which describes how the digital relief map can be used to reconstruct the palaeorelief of Cumbria and provide quantitative guidance on the potential future evolution of landforms in that area, taking glacial processes into account. This analysis is complemented by a parallel study on ice sheet development and retreat, which is described in subsection 3.4. This study addresses not only the dynamics of ice sheet growth and decay, but also the temperature and pressure fields at the base of such ice sheets, since these parameters are relevant to groundwater modelling. Finally, subsection 3.5 shows how the on-going Site Characterisation programme at Sellafield is yielding important insights on the characteristics of the Quaternary sediments and their post-glacial deformation as well as on the possibility of neotectonic movements in the area.

3.2 The Significance of Glacial Processes

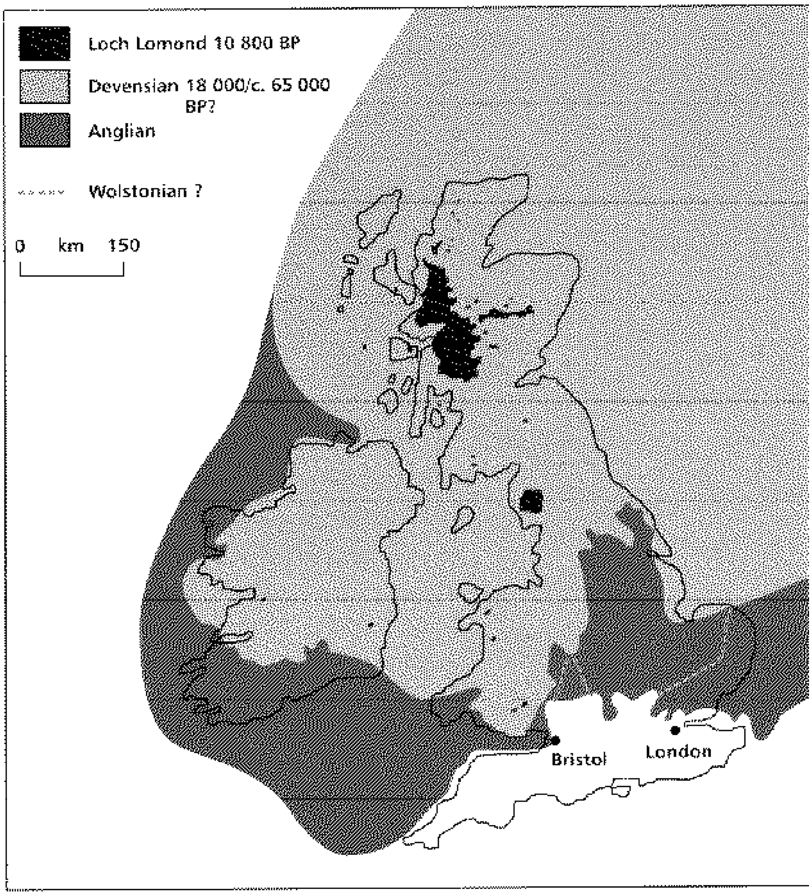
3.2.1 Glacial Episodes in Britain

During the latter part of the Quaternary the British Isles have been glaciated on several occasions and about ten more glaciations of comparable extent are anticipated over the next 1 10^6 years. The maximum extent of ice (*Figure 2*) runs from the Scilly Isles through the Bristol Channel, across to Oxford, to Finchley in North London and to the North Sea coast just east of Chelmsford [76]. The margin which does not necessarily all mark the limit of a single glaciation swings northward around the highest ground of the Cotswolds and the Chilterns.

From deep sea sediment core data (*see Box 2*), it is known that there have been eight global cold stages over the last 7.8 10^5 years. Although these eight cold stages were associated with large volumes of ice worldwide this does not mean that the British Isles were extensively glaciated in all of them. Nevertheless, it seems highly probable that upland glaciers extending at least into the adjacent lowlands occurred in all eight cold stages. Indeed the evidence indicates that glaciations extended across much of Wales and perhaps all of Scotland and northern England in at least six cold periods during the last 7 10^5 years [74].

Despite the ocean core record of global ice volume and a variety of land-based evidence, the majority of British authors currently describe the glacial record in the British Isles in terms of only two ice advances. The first is the Anglian glaciation typically dated to around 440,000 years BP [74] followed by the Devensian glaciation which reached its maximum extent around 18,000 years ago and had largely melted back to its many highland sources by about 14,000 years BP. Evidence for an intermediate glaciation the Wolstonian [77], has been reassessed (*eg* [78, 79]) and attributed to the Anglian. However other evidence has been produced to suggest that such an intermediate glaciation did occur [80, 81]. In Ireland, the record is very muddled and a consensus has yet to emerge [74] but in Scotland there is almost everywhere evidence of only one glaciation [82]. Offshore there

Figure 2 **Limits of identified glaciations of the British Isles. From A Goudie, *The Landforms of England and Wales*, Basil Blackwell, 1990.**



is good evidence of three major glaciations in the North Sea and adjacent parts of the northern Netherlands [83, 84].

This restricted view of the last 700 000 years is emphasised by the formal recognition on mainland Britain of only three interglacials prior to the present: the Cromerian, Hoxnian and Ipswichian. In terms of pollen sequences all British interglacial sites have been successfully classified as one or other of these, though the deep sea sediment core record clearly shows that others must either be missing or confused with the three named stages.

In Cumbria the field evidence mostly relates to the Devensian glaciation with sediments from former glaciations having been largely swept away with the advancing Devensian ice (*see Box 7*). Thus it is useful to set the scene for a discussion of glaciation in Cumbria by summarising what is known concerning the Devensian ice sheet.

Notwithstanding the presentation of detailed models for the growth and retreat of the Devensian ice sheet (*see, eg* [85]) it is emphasised that the dynamics of development of British ice sheets remain poorly understood [74].

- There is still disagreement about the precise limits of the Devensian ice but in general the line lay from southern Ireland across to southern Wales northwards along the Welsh marches to the west of Birmingham and the western Pennine margin, across the Vale of York and then round the margin of the North York Moors and down the eastern coast of England to northernmost Norfolk. Opinions have varied over time about the relationship with the Scandinavian ice sheet; some authors interpret the offshore evidence to suggest separation, others suggest the ice sheets coalesced. Currently majority opinion favours separation, but the issue is probably not as clear cut as some authors suggest and glacial reconstructions favour coalescence in the northern North Sea basin.
- The lobe extending to the Wash has caused debate. It has been ascribed to the influence of confluent Scandinavian ice hut more recently to a surge lobe with a low surface profile as a result of sub-surface water and/or a deformable bed. Recent work has adopted the low profile thin ice deflormable bed model much more widely and earlier reconstructions of British ice sheets modelled on the profiles of Antarctic or Greenland ice sheets are no longer tenable. Indeed it has recently been suggested that the Scilly Isles still is of Devensian age implying a long lobe reaching right down the Irish Sea. An extreme view of the collapse of this lrish Sea lobe with high sea levels leading to rapid collapse has been presented by Eyles and McCabe [86] but the relevant evidence of a high sea level stand has also been interpreted in terms of a terrestrial glacier containing reworked marine sediments [87].
- The western northern and eastern limits of the Devensian ice are not well known. Because of the lower sea levels existing at the time of maximum ice sheet extent much of the ice margin was on dry land, but the evidence now lies beneath the sea. In the far north and probably also in the northwest the ice is likely to have reached the sea and spread out as a floating ice shelf. In the North Sea the accepted limits of the Devensian ice sheet have recently been challenged on the basis of the observed distribution of subglacial or buried valleys [88].

7 A NEW INTERPRETATION OF GLACIAL BRITAIN

Publication of the offshore geological maps, scale 1:250,000, by the British Geological Survey has allowed estimation of the volume of Quaternary sediments on, and at the margin of, the continental shelf. The total volume is of the order of 80,000km^3. Estimates of the volumes of glacial deposits left by a single glaciation are 4,000km^3 on the present land surface and up to 8,OOOkm^3 on the drowned continental shelf. It is clear that, on this basis, the two (or possibly three) glaciations recognised on the British land surface cannot account for the erosion of material from the land and the continental shelf and its transport to the areas of deposition towards the shelf margins. Something like six or seven major glaciations (or even more smaller events) must have built up the Quaternary sediments lying offshore. Each of these ice advances has removed virtually all the deposits of its predecessor and moved them to build up a wedge of deposits on the edge of the shelf. During decay of the ice sheet from its maximum extent, glacial erosion has created an uneven and incomplete layer of till and associated meltwater deposits averaging some 15 - 20m thickness. In the subsequent non-glacial period, this has been dissected by rain and rivers, eroding an average depth of about 12m from areas with drift cover. Where the older (Anglian) glacial deposits survive south of the Devensian limit, an average depth of almost 17m has been removed from drift-covered areas. It is estimated that, for both Anglian and Devensian glaciations, the original thickness of drift in areas where it was deposited was close to 27m.

It is necessary to conclude that the surviving deposits of each glaciation are swept forward by the next ice advance if the offshore wedge of Quaternary deposits is to be built up to the observed total of some 80,000km^3. If older drifts were reworked with only limited forward transport to produce the new drift layer; then many more separate glaciations would be required to accumulate the 80,OOOkm^3 volume lying offshore. The sweeping clean of the rock surface by the advancing ice, followed by the creation of a new drift layer from eroded rock to be exposed by retreat, has the advantage that it accounts for the apparent simplicity of the land record. At only a few unusual sites are older glacial and interglacial sediments protected from erosion to allow the establishment of a chronological sequence on land. Over most of the area covered by the last (Devensian) ice sheet there is evidence of only a single glaciation; all older sediments have been destroyed and removed.

The accumulated deposits offshore represent an average depth of erosion, for both the present land area and the continental shelf, of 130 - 160m, the lower figure if older rocks are involved, a value nearer the higher figure if, as seems likely, the erosion was predominantly of unmetamorphosed sedimentary rocks. This cumulative pattern of glacial erosion has modified the uplands to produce a set of landforms long attributed to the work of ice. These include glacial troughs, lakes in closed rock basins, hanging tributary troughs and glacial corries (cirques).

However, careful measurement of the eroded volumes represented by these characteristic landforms shows that only in the most intensely eroded mountains do they represent average depths of erosion of more than 100m, and in most glaciated uplands the figure is far lower. Thus, the dissection of glaciated mountains cannot account for the total erosion accomplished in the Quaternary period.

This implies that erosion has been more effective on the weaker rocks flooring the major lowlands and much of the shelf offshore. This is not unexpected; the resistant rocks of the glaciated uplands bear remarkable testimony to the power of glacial erosion, but it must be anticipated that weaker rocks have suffered even more. Furthermore, the drift cover is predominantly composed of weaker sediments transported relatively short distances from the source rocks. This reflects the erosional and depositional work achieved by the most recent ice advance where it occurred, but in no way indicates the cumulative effect of successive Quaternary glaciations. These have dissected many of our uplands, but achieved more general and widespread denudation of the lowlands on our less resistant rocks, and must be regarded as the main agent achieving surface lowering there. Over the glacial phase of the Quaternary Period, overall rates of erosion for the whole land surface, but especially in these lowlands, greatly exceed those of unglaciated Britain.

All these remarks relate to the maximum extent or collapse of the Devensian ice sheet and indicate considerable uncertainties in the nature and maximum extent of the ice. The earlier phases of development of the ice sheet are even less well known, the evidence having been removed or obscured by later stages of development. However, to an extent, the very earliest stages are likely to have been mirrored by the events of the Loch Lomond stadial, at around 1 1,000 years BP, when climatic conditions were fully glacial and it was only the short duration of the event (< 1000 years) which limited ice sheet growth . During this episode, at least 64 corrie glaciers formed in the Lake District with a total area of 55 km^2, and the snowline dropped to an average elevation of 540m [89]. During this episode a true ice cap developed in Scotland of sufficient volume to cause renewed isostatic depression, while in Ireland small corrie glaciers reformed. In respect of glaciations earlier than that of the Late Devensian virtually nothing is known except in the case of the Anglian which was more extensive than the Late Devensian glaciation.

3.2.2 Evidence of Landform Change

There are two main lines of evidence about landform changes brought about by glaciation the erosional features of the uplands (and in places of the lowlands) and river diversions (both major and minor).

By their nature erosional landforms are notoriously difficult to date and the cirques, troughs and rock basins of the uplands have been eroded in several successive glaciations with long periods without ice between [74]. The effects of glacial erosion on lowland Britain are less easily recognised. However a consensus has developed that The Wash and The Fens are the result of erosion during the Anglian advance and similar arguments have been advanced for the Vale of Belvoir [74]. It seems likely that the Vale of York was lowered by ice action whilst Gresswell [90] has described the Dee and Mersey estuaries as lying within intrusive troughs formed as ice rode up southwards from the Irish Sea basin. It is thought that much of the Cheshire Plain has been reduced in level in the same way [74]. The low elevation of the crest of the Chalk outcrop east of The Fens and the absence of anything like a normal escarpment is also regarded as the work of ice [74].

The southward advance of successive ice sheets has brought about major changes in the river network of the British Isles. Most of the major diversions were accomplished in earlier glaciations but the Devensian advance is considered to have diverted the upper River Severn through the Ironbridge Gorge above Bridgnorth [74] Earlier diversions southward include those of the Thames and Yorkshire Derwent, while the River Trent between Nottingham and Newark preserves evidence of an ice marginal route as it cuts obliquely across the dip-slope of the Triassic rocks [74]

In order to quantify the degree of landform change caused by glacial action, estimates have been made of the original (and present) volumes of till and associated glaciofluvial drifts in and around the British Isles. Overall, there is good evidence that each major ice advance sweeps away the existing drift cover moving the bulk of it to the edge of the continental shelf, and erodes an average just under 20m of bedrock to produce a new drift layer averaging about 27m depth where it occurs. These glacial deposits are attacked by rain and rivers after deglaciation, and it is estimated that prior to the next ice advance almost half of this is eroded. Removal is complete along all major river valleys and where the original drift thickness was small, whereas there is very little surface 10wering across many of the broader interfluves [74]. More details of this new interpretation of Glacial Britain are given in Box 7.

Thus in this interpretation, glacial processes are anticipated to result in an average lowering of the Cumbrian land surface by about 200m over the next one million years. However, the highly incised nature of the current land surface as well as the relief contrast between the uplands and the coastal lowlands, suggests that significant spatial variations in the degree of lowering will exist. To investigate this possibility, a model is required of how the land surface has evolved to its present form and of how it may evolve in the future.

3.3 Quantifying Landform Evolution

As has been commented elsewhere [91], there are many factors affecting the large-scale relief of the British Isles: rock type and geological structure, Tertiary (and perhaps contemporary) uplift, the impact of glaciation and other styles of past erosion, the overall drainage pattern and the distance to the sea (both present and past) must all he included. There may also be others of great significance that have not yet been identified. At an early stage in the development of the NSARP biosphere sector, it was decided that a relatively simple database of some of these variables would provide a body of information that could be analysed to throw some light on the relative importance of these various factors in different contexts. Compilation of this database proved to be a time-consuming and labour-intensive exercise, hut is now sufficiently extensive for a wide range of analyses to be performed.

The database uses the 1 km squares of the National Grid, and the northern England/southern Scotland area, which is complete, covers 61,120 km^2 of land. Offshore areas are also included, with a reduced set of variables, so that the total area covered is about 130,000 km^2 extending as far south as a line from mid-Wales to the Wash. Data from northern Scotland are currently being added. For each grid element on land, the data recorded comprise the highest and lowest altitude to the nearest metre, the geology (both age and lithology) for the dominant outcrop of each square, the river distance in km to tidal water, and the local variation of gravity from its standard value. From this considerable database, it has proved possible to establish a number of general relationships between river distance, geology and height above sea level. In particular, it has proved possible to classify the many different outcrops into five bands of varying resistance to erosion) where the primary indicator of resistance is the ratio of the mean height of outcrop and the mean river distance. Where the area of a rock type (classified by age and lithology) is reasonably large (> 100 km^2) and not restricted to a particular locality, the resistance classification is robust, hut for smaller or unusually located areas the class may prove to be incorrect once a wider area is available for analysis.

In considering the use of the digital relief map in analyses specific to Cumbria, it is first relevant to note that trough volumes in the Lake District upland have been measured using published topographic maps. The total volume is about 220 km^3, equivalent to an average reduction in surface elevation of 120m. Though the same method cannot be used to estimate glacial erosion in the surrounding lowland, the magnitude of the reduction in surface elevation might be expected to be rather larger because:

- The rocks are weaker and hence more susceptible to erosion;
- The average amount of glacial erosion inferred for the British Isles is 130 to 160m *(Box 7)* so that if an upland area of intense glacial erosion such as the Lake District contributes only 120m, lowland areas on weaker rocks must contribute more.

The simplest analyses that can be undertaken using the digital relief map are based on the reconstruction of palaeosurfaces. Three such surfaces are readily identifiable, of which the first two are particularly relevant to estimating erosion during the Quaternary:

- The summit surface constructed using smooth contours based on the highest summits In the area;
- The present relief;
- The structure of the Upper Palaeozoic and younger rocks which surround the Lake District,

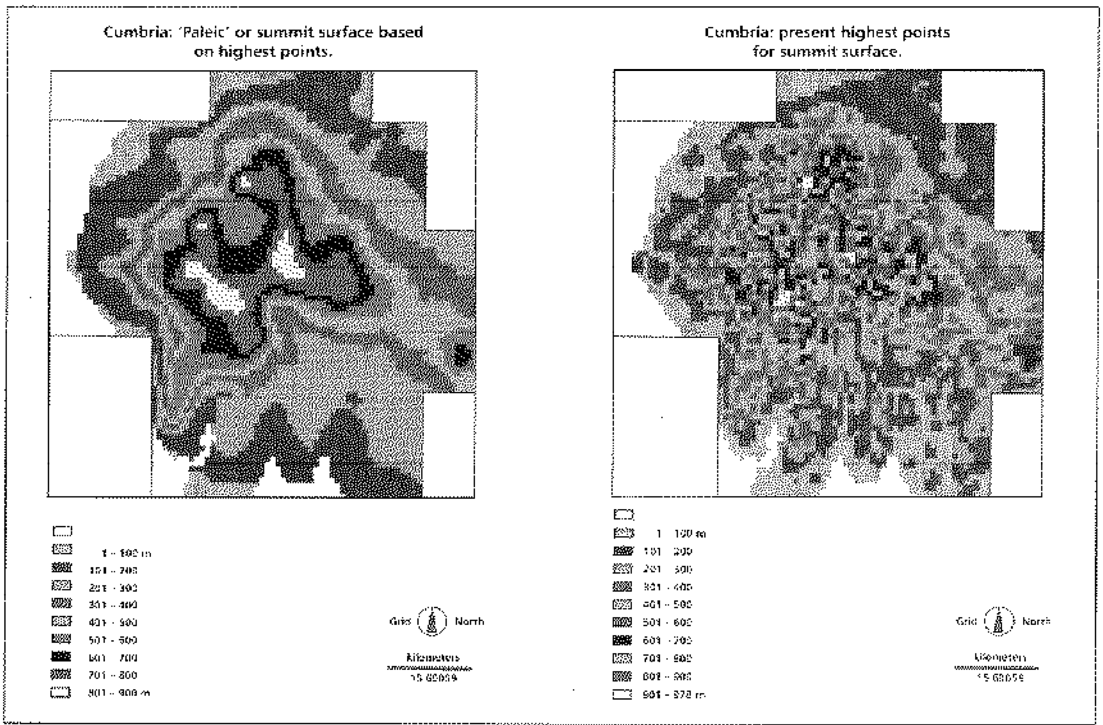
which may be projected towards the centre to complete a domal form.

As the reconstruction of the shape and height of the dome implied by the dip of the surrounding younger rocks (notably the Triassic sequence) has yet to be completed, the analysis undertaken to date is based on the first two of these surfaces (*illustrated in Plate 2*).

Overall, the erosion below the summit surface to the level of the present relief, for the area shown in Plate 2, is 136m, with half the values lying between 32m and 152m. It is significant that the average depth of 136m is no more than the average value of about 1 50m calculated for northern (glaciated) Britain during the last 700,000 years of the Quaternary. However, of even greater interest is the observation that this figure (which is for total lowering) is not substantially larger than the value of 120m based on trough volumes only. This indicates that a very high proportion of the volume removed from below the summit surface represents the effects of glacial erosion, and strongly suggests that the summit surface forms a reference for the overall landform of Cumbria at around the Quaternary/Tertiary boundary.

Thus, in reconstructing an early Quaternary form for Cumbria, it is appropriate to envisage an upland similar in form, if not in elevation, to the summit surface shown in Plate 2. This would have been surrounded by a ‘lowland’ of weaker rocks probably about 200m above the present surface, taking account of their greater susceptibility to erosion and the constraint that the average depth of glacial erosion for the area as a whole should be

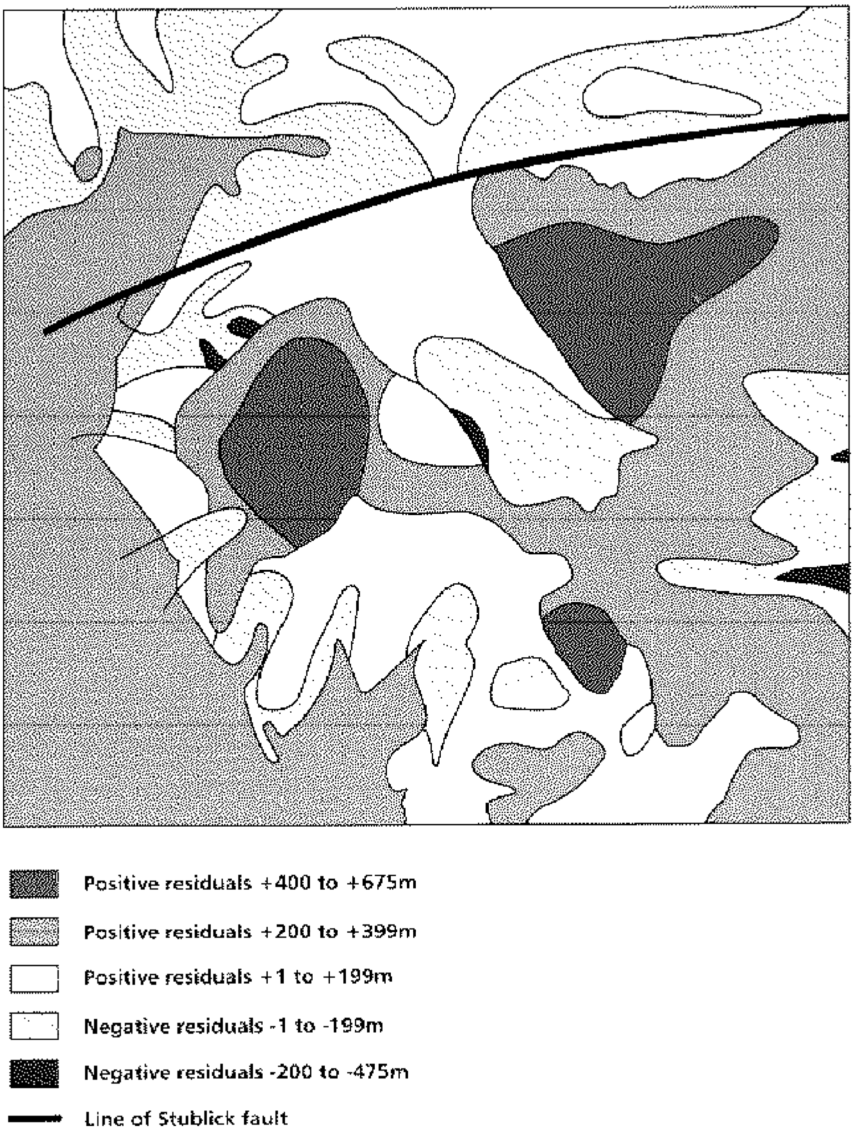
Plate 2: Present topology and summit palaeosurface of Cumbria



about 150m to be consistent with overall estimates for northern *Britain (see subsection 3.2.2, and noting the particularly intense glacial erosion of this area inferred from the form of present-day landscape*). However, it would be impossible to remove so much rock in such a short time without activating compensatory isostatic uplift, which will have been of the order of the average depth of erosion. This uplift has to be used to move the reconstructed palaeosurface downward. Thus, the most probable reconstruction using this evidence is that, during interglacial episodes of the early Quaternary, the land surface at the level of the highest summits in the central area of Cumbria, on the Lower Palaeozoic rocks, reached altitudes above sea level of about 150m less than at the present day. The highland would have been surrounded by lower ground, as today. However, given the former generally greater height of the lowland, it is possible that the coastline was further away from the Lake District than it is today and that the ring of encircling Upper Palaeozoic and Mesozoic rocks was wider.

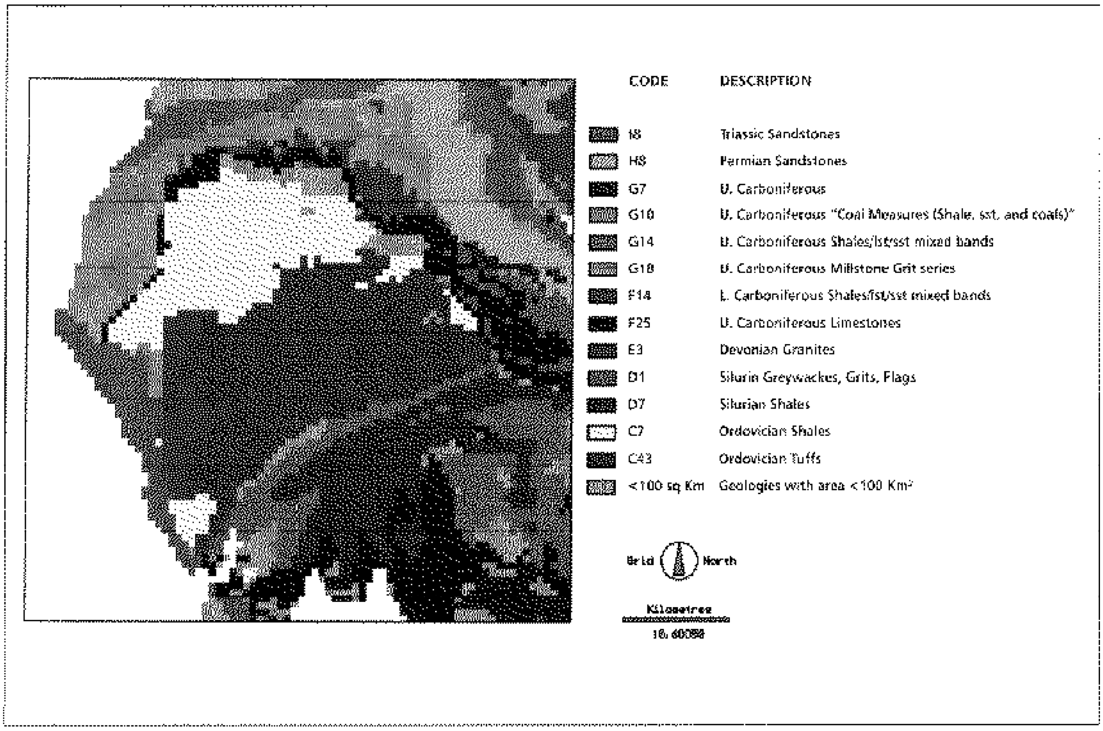
An alternative approach is to compute residual differences between observed and expected heights, making allowance for the varying resistance of different types of geological strata and for varying river distance from the present-day coastline. Smoothed results of this approach are shown in Figure 3. In this figure, the large positive residuals for the Lake District upland relate to the ridges between the glacial troughs, with the troughs themselves showing smaller positive or negative residuals. Outside the Lake District, large areas show negative residuals in the range -1 m to -199m and considerably smaller areas show negative residuals of -200m to -450m. The pattern of these negative residuals and the total lack of correspondence with the pattern of geological outcrops (*Plate 3*), suggests

Figure 3 Height residuals for Cumbria obtained from anaylsis of the data available in the digital relief map.



that, like the troughs within the lake District itself, these are areas lowered by ice-driven erosion. The one partial exception is the generalised boundary that continues from the north side of the Lake District through Carlisle to Haltwistle. This would seem to be linked to major structures that have

Plate 3: Geological outcrops in Cumbria



this trend, and in particular, to the line of the Stublick fault.

On the basis of this analysis, a number of eroded basins can be identified around the Lake District, some of them open to the Irish Sea, with the most negative residuals close to the margin of the upland. A good example is Wastwater, where the lake bottom descends to below sea level. In all cases, the basins extend far into the Lake District, supporting the view that they are due to deep erosion by ice.

Overall, the residuals show basins with departures from the average for similar rocks and river distances of between -200m and -450m, with ridges of Triassic sandstones and similar outcrops exhibiting positive residuals of about 100m. Thus, the residual relief range is about 550m, compared with a residual relief range of about 200m for similar rocks beyond the glacial limit. This may perhaps be attributed to the excavation of the deep basins by ice, with far less erosion on the ridges.

From this analysis it is not possible to estimate the amount of erosion of the ridges, but, even if it were negligible, the maximum depth of ice erosion in the basins would be 550m. In fact, estimates of the onshore and offshore drift volumes for the area indicate that the Devensian glaciation generated approximately 53m depth of drift, corresponding to the erosion of 39m of rock. Assuming seven major glacial episodes during the Quaternary, this corresponds to an average of 275m of erosion. This implies that the ridges could have been lowered by ice by about 1 00m and that the maximum depth of glacial erosion in the basins could have been about 650m.

In summary, it appears that the relief contrast between the Lake District and the surrounding lowlands has been increased by Quaternary glacial erosion. This reached an average depth of only 120m on the lower Palaeozoic rocks (though far more in the glacial troughs) and the highest ridges were largely spared. On the surrounding rocks, erosion was of the order of 100m on the higher ground, and reached 650m in the deeper glacially eroded basins. Yet although ice has achieved a rapid evolution of the landscape in a relatively short space of time, it has done no more than continue a process of differential erosion that must have been going on throughout the late Tertiary with rain and rivers as the dominant agents. Rather similarly, although the rapid unloading achieved by erosion in the Quaternary has speeded up the process, the uplift of the whole area (upland and western lowland alike) has continued from Tertiary times.

Thus, the relief contrast we see today requires no structural discontinuities between highland and lowland on the western side. It could be that dislocations occur to the north and less certainly to the south. On the north, the elevation residuals suggest a discontinuity aligned WSW-ENE, along the line of the Stublick fault. There is no obvious indication of a dislocation on the southern side, though there may be a discontinuity somewhere along the northern margin of Morecambe Bay and then ENE towards Sedburgh.

3.4 Modelling Ice Sheets and Their Effects

The analysis provided in subsection 3.3 demonstrates that ice-driven erosion has had a major impact on the relief of Cumbria (both the Lake District upland and the western coastal lowland) over the last one million years. Effects of comparable magnitude are anticipated over the next one million years. However, in addition to their erosive effects, ice sheets cause substantial isostatic depression of the land surface and also can change markedly the boundary conditions appropriate for groundwater modelling. It is, therefore, appropriate to develop quantitative models of ice sheet growth and decay which can be used to assess the potential impacts of future glaciations on Cumbria in general and on the Sellafield area in particular.

Considerable effort has been expended in the development of mathematical models of ice sheet growth and decay, but consideration of the literature [92-98] gives rise to a concern that existing models may be inadequate for representing evolving conditions in the Sellafield area. Specific weaknesses are summarised below.

- Existing models of large ice sheets are essentially uncoupled from the thermomechanics governing the evolution of the atmosphere, oceans and Earth's crust; boundary conditions are prescribed at the interfaces, whereas in reality interactions at the interfaces influence the evolution of both the ice sheet and the environment in which it develops.
- Conditions at the base of a grounded sheet are far from clear; for instance, the degree of basal melting, and the relationship between tangential velocity and tangential stress.
- Ice sheet evolution over large areas must be influenced by the undulation topography, crustal deformation, and the essentially three-dimensional nature of the flow. The reduced models that are currently used are really only applicable to small slope topography with prescribed bed form, and the numerical algorithms for vertically plane (or axisymmetric) flow. Depth integrated models involve arbitrary, doubtful, approximations.
- The treatment of evolution as sequences of steady states is a useful approach, but can lead

6

ENTWIFE AND ITS CAPABILITIES

ENTWIFE is a computer program, produced by AEA Technology, for solving non-linear partial differential equations of elliptic type using the finite element method. ENTWIFE was originally developed to solve laminar fluid flow and heat transfer problems, but it was recognised that the techniques could easily be extended to a more general class of problems. This was achieved by developing a preprocessor called ENTCODE which is based on the REDUCE algebraic programming system. The input to ENTCODE is a simple symbolic description of the governing partial differential equations and boundary conditions; the output is the set of FORTRAN subroutines required by ENTWIFE to define the governing set of equations and their low-order derivatives. The manual evaluation and coding of these derivatives is a laborious and error prone exercise - the ENTCODE preprocessor is both fast and accurate.
A coordinate transform technique is used an ENTWIFE to solve free-boundary problems. The unknown region, bounded by the free boundary, is mapped onto a fixed domain using an orthogonal transformation. The governing equations are expressed in terms of the transformed coordinates and are solved, together with the equations defining the mapping, on the fixed domain. This technique has been applied with great success to the problem of the free-surface flow of an incompressible, viscous fluid down an inclined channel with two smooth bumps in its bed. The results obtained using ENTWIFE were compared with laboratory measurements of the height of the free surface above the bed of the channel due to Pritchard, Scott and Tavener. Figure A shows a comparison of the computations with the experimental measurements. The level of agreement is very good, particularly when it is borne in mind that there are no adjustable free parameters in the model.

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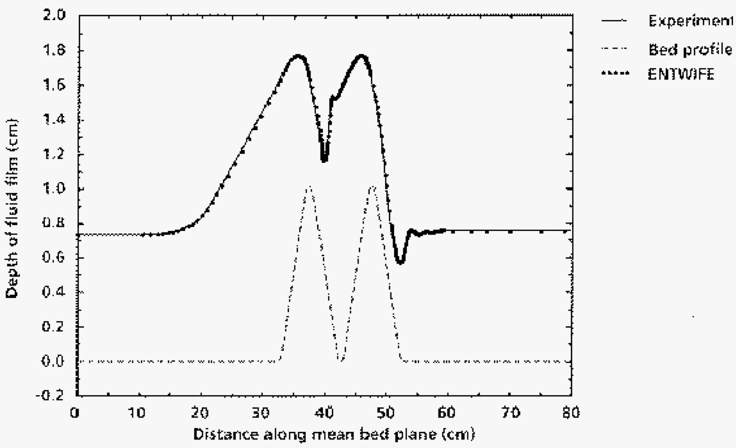


Figure A: Comparison of ENTWIFE computation with laboratory experiment for flow of a viscous fluid down a perturbed inclined plain. The depth of the fluid film is plotted against distance along the plain.

to an entirely wrong picture. Thus, it can be shown that evolution from an equilibrium state under a sudden change of surface conditions can result in the profile changing in an opposite fashion to that suggested by the equilibrium state for the new conditions.

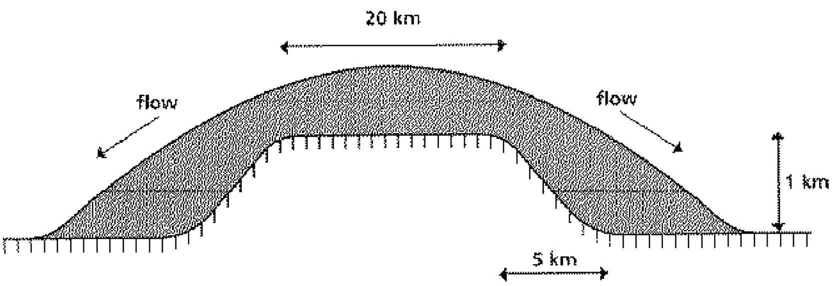
In view of the doubts which exist with respect to the adequacy of existing ice sheet models, a model comparison exercise has been instituted within the NSARP to compare results from a reduced model appropriate to small slope topography with a numerical model that does not include this approximation. In the first instance, the two models are being compared for an idealised radially symmetric 1-D case in which an ice dome develops over an upland area of dimensions comparable to those of Cumbria (*Figure 4*). In this study, the ice dome is assumed to develop over a bed which does not change its shape with time, i.e. isostatic effects are neglected, and prescribed basal sliding laws and temperature-viscosity relationships are assumed. It is anticipated that the significance of bed deformation and alternative sliding laws in overall ice-sheet development will be investigated in future studies.

The radially symmetric reduced model, while based on approaches already available in the literature (*see, eg* [92-98]) requires some analytical developments which have been put in hand. The numerical model that is being developed is based upon the ENTWIFE program developed by AEA Technology for the modelling of general free boundary problems [99] (*see also Box 8*).

As noted above, the effects of a developing ice sheet include crustal deformation and erosion. Crustal depression and recovery with ice sheet loading and unloading has been studied in some detail for the British Isles, with account having also been taken of the loading of the sea floor by water. A useful summary of the current state of the art has been provided by Lambeck [100].

"The occurrence of raised and submerged shorelines of Scotland, England and Wales is well documented and has been qualitatively understood in terms of two components; the crustal rebound in response to the melting of the late Pleistocene ice sheet over the British Isles and the rise in sea level resulting from the quasi-simultaneous melting of the more voluminous ice sheets over North America and Europe. To this have to be added smaller but still significant contributions from the rebound of nearby Fennoscandia and from the loading of the sea floor by the water load. Models of this glaciohydro-isostatic rebound require a knowledge of both the history of glaciation and deglaciation and of the Earth's response to changes in surface loading. The application of the models has often been limited by the difficulty of separating the uncertainties introduced by an inadequate knowledge of the ice history and of the Earth theology, but by matching model predictions with observations, it becomes possible in some circumstances to separate these two sources of

Figure 4 **Idealized 1-D model being used to study ice sheet growth and decay**



unknowns and to develop consistent rebound models. This is the case for the British Isles where there is a reasonable distribution of Holocene sea-level observations from sites around and within the limits of glaciation, including sites quite close to the former centre of glaciation. For this region the retreat of the ice over land appears to be reasonably well established from a variety of field evidence but the retreat of ice over the adjacent shallow sea floor is more controversial. Also estimates of the thickness of the ice sheet vary by up to 50% from one model to another and as a result the various published models can differ significantly in the estimates of total ice volume. Nevertheless, it has been established that, because of the nature of the distribution of the sea level observations, a partial separation of parameters describing the ice history from parameters describing the Earth response can be established and that rebound models can be established that are consistent with the sea level data, with the geological evidence, and with rebound analyses for other regions around the globe. Such models also provide a basis for reconstructing palaeo-shorelines in the offshore region and for constraining models of Holocene and Late Devensian coastal evolution. In addition, the models can be used to place some age constraints on some of the older shorelines and platforms of Scotland whose ages have only been indirectly inferred, and to test some of the correlations proposed for shoreline fragments around Scotland, northern England and Ireland."

Lambeck [100] emphasises the good agreement between observations and theory, but also notes that there remains room for improvement, and points out that a potentially important area for further investigation is the northwest coast of England, the Isle of Man and the Solway Firth area, where the model predicts that, for a brief period after local deglaciation, shorelines could have formed that would now be above sea level. This matter is currently under active investigation in the Nirex Site Characterisation programme (*subsection 3.5*)

3.5 Status of the Research, and its Relationship to Assessments and to Site Characterisation

The research undertaken to date has emphasised that glacial processes are of potentially great significance to the post-closure radiological performance of a deep geological repository at Sellafield. Thus, a single glacial episode is sufficient to totally remove the existing drift deposits and regenerate them by eroding, on average, 20 to 30m of the underlying rock. Over the next one million years, it is anticipated that ice-driven erosion will tend to accentuate further the relief contrasts within the Lake District upland, but, more particularly, between the upland and the adjacent lowland plain. Further analyses using the digital relief map are being undertaken, with a view to confirming the preliminary palaeoreconstructions reported here and extending the work to providing projections of possible future relief surfaces. In parallel, the ice sheet modelling studies should yield a good indication of whether a reduced version of the full ice sheet model can be applied to Cumbria. In any event, both the reduced model and the full numerical model will be available to generate temperature and pressure fields at the base of the ice sheet for use in transient groundwater modelling studies, to provide guidance on the potential influence of ice sheet development on the underlying groundwater flow regime. This is likely to involve an intermediate stage of investigating the coupling of ice sheet development and bed deformation along the lines already explored by Lambeck [100].

9 MAPPING QUATERNARY SEDIMENTS IN THE VICINITY OF SELLAFIELD

On-shore Quaternary sediments at Sellafield have been mapped by the British Geological Survey (BGS) on the basis of existing documentary information, walk-over surveys, trial pit logging and sampling, and geophysical investigations. The geophysical techniques used have included ground-probing radar, conductivity traversing, apparent resistivity sounding and shallow seismic refraction. Pit observations comprised conductivity and gamma logging, complemented by photography and filming with closed circuit television.

Ground-probing radar has proved successful in distinguishing between the major lithological sequences (clays, sands and gravels of various grade), but its penetration is limited to about 7m in dry, resistive sediments and some 2m only in the presence of clays and diamicton. Conductivity and resistivity surveys have yielded limited data complementary to those obtained by ground-probing radar. Seismic refraction at a limited number of sites indicates only a small range of P-wave velocities and it is unlikely that this technique alone could characterize the Quaternary sequence. However, the technique has successfully indicated depths to both bedrock and the water table, down to depths of about 30m. Preliminary investigations have shown that detailed information on faulted structures could be obtained through a combination of P- and S-wave seismic tomography in areas where boreholes may be drilled.

On the basis of the work undertaken to date, it has been possible to distinguish principal Quaternary domains defining landform and sediment assemblages. In particular, glacitectonically disturbed and glacially over-ridden domains are recognised on the basis of structural and landform association observations.

Other recognised Domains include:

- Solid (Bedrock) at or near surface
- Thin till deposits (usually <5m thick) on rock
- Alluvial deposits overlying possible Postglacial sequences
- Pre-Holocene Valley Infill deposits (including sandur and deltaic deposits)
- Glaciolacustrine deposits
- Possible pre-Late Devensian Quarternary sequences (concealed by younger surficial deposits)

Where possible, the Domains have been subdivided into their main lithologies. Stratigraphically, Glaciofluvial deposits, both underlain and overlain by till sequences, are commonly identified.

Offshore, considerable reliance is placed on high-resolution seismic data, which show a well-defined stratified sequence of sediments. Correlation of the offshore and onshore sequences remains conjectural, but is currently being attempted using various unconformities as markers with chronostratigraphic significance. The chronostratigraphy is, however, as yet poorly constrained. The approach being adopted is to use available seismic, borehole, trial pit and other geological information to construct 2-D transects perpendicular to, and crossing, the present-day shoreline.

In order to characterize the Quaternary deposits at a resolution relevant to detailed near-surface hydrological modelling, extensive use is being made of the many borehole records that exist. For selected locations, the borehole density is sufficient to attempt model-independent reconstructions of the 3-D characteristics of the deposits.

However, it is emphasised that a major glacial episode at Sellafield is not expected to occur until around 60,000 years AP and that its intensity may be significantly mitigated as a consequence of the enhanced greenhouse gas emissions occurring at the present day (*Section 2*). For these reasons, it is appropriate to give significant attention to the structure and properties of existing drift deposits in the Sellafield area, since these have been demonstrated to have a significant effect on the post-closure radiological performance of a repository through their role in controlling the flow and mixing of meteoric and ground waters (*see Section 4*)

Also, the existing drift deposits onshore and offshore at Sellafield provide extensive evidence on the history of the area subsequent to the Last Glacial Maximum and this evidence is directly relevant to assessing how the environment may develop subsequent to future glacial episodes.

Finally, these post-glacial drift deposits may provide clues to any post-glacial fault movements in the area, either through fault displacements which propagate through the sediments and/or through sediment convolutions that can be interpreted as evidence of seismically induced liquifaction (*ie seismites* [101, 102]).

Taking all these considerations into account, Nirex has put in place a Quaternary component of the Site Characterisation programme designed to:

- Map the drift deposits onshore and offshore, including provision of information on their lithology and stratigraphy (*see Box 9*);
- Characterise the hydrological properties of the drift at selected locations, in the context of an overall programme of near-surface hydrological monitoring (*see Box 15*);
- Identify and characterise any areas where they may be evidence of significant post-glacial movement along faults.

This component of the Site Characterisation programme includes:

- Walkover mapping studies, including detailed examination of existing drift exposures;
- Excavation of pits to a depth of about 3.5m at selected locations to characterise the lithology and hydrcalogical properties of the upper part of the drift;
- Construction of boreholes for lithological and hydrological studies, and for exploring potential neotectonic features;
- Analyses of data from existing boreholes and seismic studies to construct detailed 3-D maps of the drift for illustrative areas and to provide transects illustrating the on-shore to off-shore correlations of the observed deposits;
- Detailed analysis and dating of sediment cores from the Irish Sea and Wastwater to provide quantitative information on regional changes in sea level subsequent to the Last Glaciation.

More details of the work on near-surface hydrological monitoring are provided in subsection 4.4.

4 Simulating Radionuclide Transport at the Catchment Area

4.1 Status of the Research in 1992

As pointed out in the previous review of the NSARP biosphere sector [4], the near-surface hydrological system is a major factor in determining the distribution and transport of radionuclides in the biosphere following their emergence from the geosphere. In particular, there is a need to determine the degree to which radionuclide concentrations in groundwaters entering terrestrial catchments are diluted by mixing with meteoric waters, and the potential for reconcentration of radionuclides by sorption to soils and uptake by plants and animals.

In order to explore these issues, Nirex makes use of SHETRAN-UK, which is a derivative of the European Hydrological System (SHE) model [103, 104], enhanced to include radionuclide transport in the solute and sediment phases (*see Box 10 and Plate 4*).

The SHE is a physically based, spatially distributed, catchment flow modelling system developed jointly by the Danish Hydraulic Institute, the British Institute of Hydrology and SOGREAH (France).

The SHE is physically based in the sense that each of the components is modelled either by finite-difference representations of the partial differential equations of mass, momentum and energy conservation, or by empirical equations derived from independent experimental research. Spatial distribution of catchment parameters, rainfall input and hydrological response is achieved in the horizontal through the representation of the catchment by an orthogonal grid network and in the vertical by a column of horizontal layers at each grid rectangle. The channel system is represented along the boundaries of the grid rectangles, with a channel link corresponding to a rectangle side.

A test application of the SHE to the Wye catchment in mid-Wales was demonstrated by Bathurst [105]. The SHE has also been tested in a variety of countries including New Zealand, Switzerland, Thailand, the United Kingdom, the United States of America, France, Denmark, Italy and Germany. It has more recently been applied to subcatchments of the Narmada basin, India [106, 107] and to snowmelt in a 40 ha subcatchment of the Reynolds Creek Catchment, Idaho, USA [l08]. Recent applications in Spain and Portugal have also been reported [109].

The sediment yield component of SHETRANUK is based on the work of Wicks [110]. It determines soil erosion and transport within the catchment, and calculates the amount of sediment outflow from the catchment. It has been designed as an overlay which takes as its input the output from the flow model. As of 1992, the original model developed by Wicks [110, 111, 112] had been applied only once, to a 33m^2 rainfall simulator plot and a 1 hectare sub-catchment at Reynolds Creek, Idaho, USA [113, 114].

It should be noted that the sediment yield and routing component of SHETRAN-UK considerably extends the work of Wicks [110, 111, 121], since it includes routing by size fraction and other modifications to account for cohesive sediment dynamics, infiltration of sediment into the stream channel bed, overbank deposition and erosion of material from stream banks.

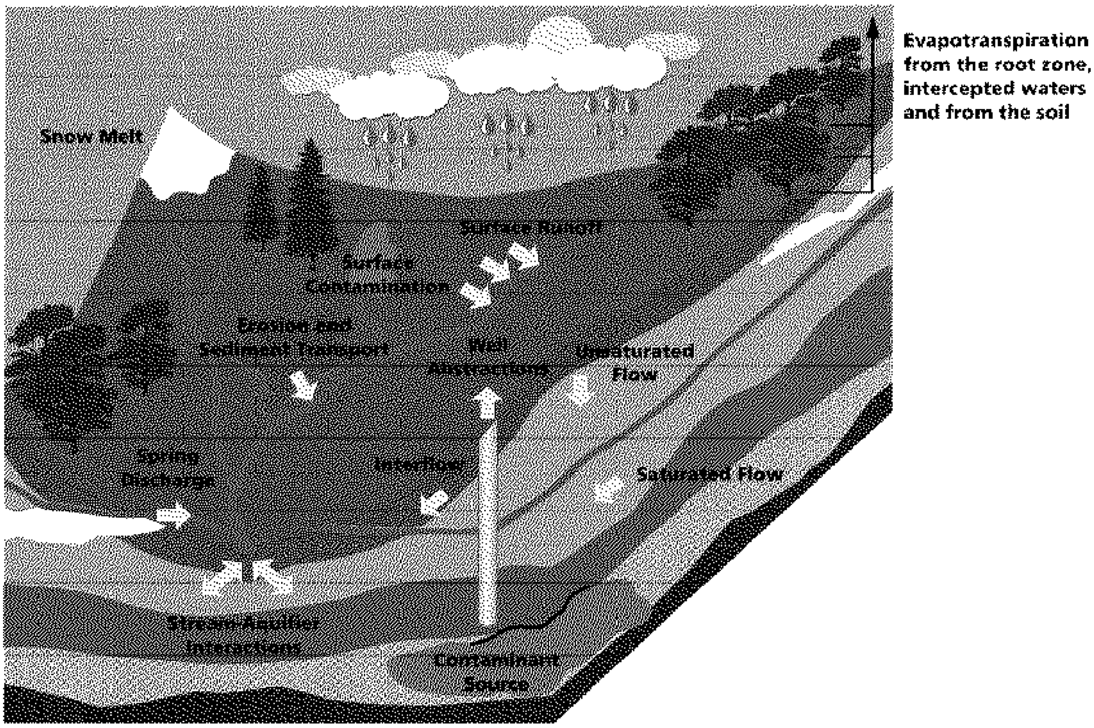
The radionuclide transport component of SHETRAN-UK iS a further overlay on the flow and sediment transport components. The basis of the transport component for the sub-surface saturated and unsaturated groundwater flow domains has been described by Ewen [115]. Having reviewed processes relevant to tracer migration in field conditions, Ewen [115] concluded that the one dimensional, two-region (mobile/immobile water) model of van Genuchten and Wierenga [116] is most appropriate for use as the basic model for contaminant migration in unsaturated and saturated soils and sediments. It is relevant to some applications to note that the two-region model reduces to a standard convection dispersion-retardation model if appropriate values are set for some of the parameters [115].

For SHETRAN-UK, the original two-region model has been extended to include extra terms for plant uptake storage and recycling radionuclide decay and ingrowth and lateral convection in the saturated zone [115].

Particular consideration has been given to the interactions between groundwater and streams. A review of this topic indicated that these interactions required explicit representation in the model. Thus, a specific stream bank component was developed to represent radionuclide migration into and within the soil in stream banks and for transfers between groundwater and streams [115]. This necessitated the incorporation of a corresponding stream bank component in the flow model which was also enhanced in respect of the representation of overbank channel flow and three-dimensional saturated zone flow.

The surface transport component of SHETRAN-UK accounts for inputs of radionuclides from dust rain and the unsaturated zone sorption to transported sediment particles, and transport in dissolved and sorbed form. For the stream channel it accounts for inputs from dust rain overland flow and bank erosion interactions with the bed material and the saturated zone sorption to transported sediment particles and transport in dissolved and sorbed form.

Plate 4: The overall structure of SHETRAN-UK



10 THE STRUCTURE OF SHETRAN-UK, VERSION 3.4

SHETRAN-UK is a state-of-the-art distributed, physically-based river catchment modelling system with the flexibility to be used in a wide range of studies related to hydrological research, water resources engineering and environmental impact assessment. The catchment to be modelled is divided into cells using a 3-dimensional mesh, and the dynamic movement and storage of water, sediments, and solutes simulated through time. The limiting factor on the size of the cells is usually computing resources. If the simulated period is a few decades, with current computers the total number of cells is limited to around 20,000, so the ground surface can be divided into 50m squares for a 1km² research catchment, or 2km squares for a 1000km² catchment. River channels are assumed to follow the mesh, and the channel network in the catchment is represented by a network of river cells, each lying along the side of one square. In practice, rectangles can be used instead of squares, and it is usual to include river banks as long thin rectangles lying on either side of each river cell. The soil and rock below each square or rectangle is divided, by the 3-dimensional mesh, into layers; various layer thicknesses are used, ranging from a few centimetres near the ground surface to a few metres for the lower regions in substantial groundwater aquifers. During a simulation, movements and storages are evaluated for each cell once per time step, with the typical step being an hour or two during dry periods, dropping to a few minutes during storms. The calculations for any cell use physical property data for the materials in that cell, so the heterogeneity within the catchment of the vegetation cover, channel network, soil horizons, rock formations, etc. can be quite fully represented.

SHETRAN-UK is a marriage between computing science, data assembly and analysis techniques, and physically based, hydrological process modelling. To create the system, the differential equations describing the hydrological processes were first determined then broken down using standard finite-difference techniques into algorithms for the cell calculations; the cell equations were then incorporated within an overall software system framework. The development of the software for the full modelling system was a substantial undertaking since it is complex and extensive, and has associated graphical tools (the SHEGRAPH system). These tools are essential in the analysis of the extensive 4-dimensional results which are produced for each simulation.

At the heart of SHETRAN-UK is an understanding of the physical processes for the storage and flow of water, and the storage and transport of sediments and solutes. The modelling system was developed within the Water Resource Systems Research Unit at Newcastle University, so research was the prime motivation, especially research into physically based process models and their integration within a coherent system. The main processes are depicted in Plate 4 of the main text, each is modelled using a physically based process equation.

By physically based it is meant that the parameters of the equation are physical properties which can (in most cases) be measured directly in the laboratory or field, so do not require calibration within SHETRAN-UK. A typical physical property is the saturated hydraulic conductivity of a rock, measured in the field using a borehole pumping test. The importance of the physical basis is that calibration is not an essential step in the use of the system, so the system can readily be used when calibration data are not available- in the study of hypothetical environmental impacts, for example. A full list of the process equations is given in Table A.

To give an indication of the capabilities and flexibility of SHETRAN-UK, a list of recent major studies in which it has been used is given in Table B.

Validation of SHETKAN-UK against field data has been a major component of the programme throughout. To 1992, attention was directed primarily to data collection for validation of the flow component, using a methodology specifically tailored to assessing the predictive accuracy of hydrological models when applied to hypothetical scenarios [171]. (A new methodology was developed as none of the validation tests in the scientific literature was appropriate in this context.) The catchments studied included snowmelt catchment (Upper Sheep Creek, Idaho, USA), a Mediterranean catchment (Rimbaud, France) and a temperate catchment (Slapton Wood, Devon, UIC). The two former studies are based on historical data for the overseas catchments, whereas the work

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Table A: Hydrological Process Equations Incorporated in SHETRAN-UK

Flow in saturated zone	Boussinesq equation (2D) (3D velocity field is inferred from the 2D results)
Flow in unsaturated zone	Richards' equation (1 D; for column below each rectangle) with a term added for plant uptake
Overland flow	Approximation to Saint Venant equations, diffusion form (2D)
Channel flow	Approximation to Saint Venant equations, diffusion form (1 D network)
Canopy interception, storage and drip	Rutter equation
Evaporation	Penman-Monteith equation (simpler alternative can be chosen)
Snowpack and melt	Accumulation and energy budget melt equation (simpler alternative degree-day equation can be chosen)
Overland sediment transport	Advection-dispersion equation (2D) for multiple size fraction transport; including deposition, and erosion by raindrop and leaf drip impact and overland flow
Channel sediment transport	Advection-dispersion equation (1 D) for multi-fraction transport; including deposition, erosion, and infiltration into the bed
Surface and subsurface solute transport	Advection-dispersion equation (3D) for multi-species transport; including adsorption, dead-space, erosion of contaminated soil, transport and deposition with contaminated sediments, plant uptake, deposition from the atmosphere, and radioactive decay
Channel solute transport	Advection-dispersion equation (1 D network) for multi-species transport; including transport and deposition with contaminated sediments, overbank transport, deposition from the atmosphere, and radioactive decay

at Slapton Wood has involved installation of equipment specifically for validation purposes to measure meteorological variables, soil moisture contents and matric potentials, and streamflows.

An important factor in using SHETRAN-UK is to have in place procedures for defining soil hydraulic characteristics at an appropriate spatial scale. A literature review on this topic was published in 1990 [118], and this has been followed up by field work at Slapton Wood and other sites to assess the practicality of the methods identified in that review [119, 120]. In addition, work has been undertaken to define transport pathways in soils using conservative tracers in con junction with intact soil cores, according to the approach described in a previously published report [112].

4.2 Model Validation

By January l 992, a fully tested version of SH ETRAN UK (Version 3.4) was available both for validation studies and for application to hypothetical catchments considered appropriate to future conditions at Sellafield (*subsection 4.4*). In addition, data suitable for use in validation of the water-flow component of the code had been acquired for three contrasting catchments and a blind validation methodology had been developed [117]

Subsequent work has included:

- Completion of the blind validation for Rimbaud;
- Use of the data from Upper Sheep Creek in validating the snowmelt component of the model;
- Collecting and analysing data at the intact core

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Table B: Recent Major Studies Using SHETRAN-UK

Project Title	Sponsors	Description	Catchments Modelled
NERC/ESRC Land Use Project (NELUP)	NERC/ESRC	Evaluating effects of rural land use change in the UK	Assessing hydrological consequences of land use change in subcatchments of the River Tyne
A Comprehensive Forecasting System for Flood Risk Mitigation and Control (AFORISM)	European Commission	Analysis of model sensitivity to spatially distributed rainfall inputs	Reno catchment, Italy
EUREKA	DTI, Thames Water, European Commission	Integration of SHETRAN in a Decision Support and Geographical Information System for river basin management and environmental impact assessment	Kennet catchment, (tributary of Thames)
Mediterranean Desertification and Land-Use (MEDALUS)	European Commission	Evaluating hydrological and sediment yield effects of land degradation and climatic variability in Mediterranean dryland areas. Assessing the effectiveness of mitigating measures against land degradation	Cobres catchment, Portugal; Mula catchment, Spain; Agri catchment, Italy
DM2E. Simulating Impacts of Vegetation Loss	European Commission	i) Simulation of impacts of forest fire on hydrological regime and sediment yield ii) Simulation of 'badlands' gully erosion, and its control with vegetation	Rimbaud and Draix research catchments, southern France

and field plot scales for validating the contaminant transport component of the model.

Validation against the field data from Slapton Wood is currently on-going, having been deferred because of the importance of completing an initial series of hypothetical catchment studies (*see subsection 4.4*). The studies on Slapton Wood, when complete, will provide a substantial validation of the subsurface component of the code, in consequence of the extensive and varied dataset acquired at that site (*see Box 11*).

Because the data from Upper Sheep Creek were used only to validate a single component of the model, while successful, they are of limited interest. Thus, the remainder of this subsection concentrates on the validation studies for Rimbaud and on the core and plot experiments which are now providing data for validation of the contaminant transport component of the model.

4.2.1 Validation of the Water-flow Component of SHETRAN-UK for a Mediterranean Catchment

The selected catchment is the 1.4 km^2 Rimbaud headwater catchment of the Real Collobrier, near Toulon in southeastern France (*Figure 5*). The Réal

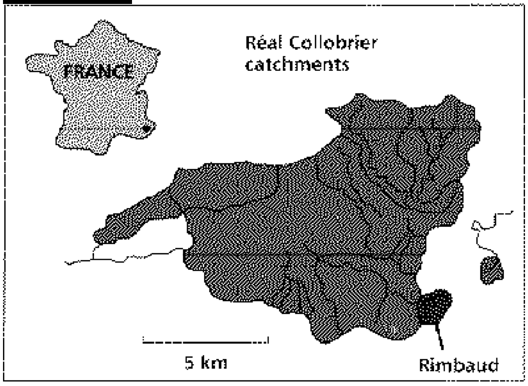
Collobrier constitutes a collection of neighbouring and nested research catchments administered by the Centre National du Machinisme Agricole du Genie Rural des Eaux et des Forets (CEMAGREF), with which a close working relationship has been established.

The catchment was selected for validation purposes because:

- It has a long (more than 25 year) record of meteorological and discharge data;
- Its soil and vegetation distributions are relatively homogeneous;
- There is relatively little topographic variation (470-620m) so that the spatial variation in precipitation is likely to be small;
- It has a well-defined impermeable bedrock (gneiss);
- Information on soil hydraulic properties was already available;
- One of the two meteorological stations in the Real Collobrier is located immediately next to the catchment so its evaporation characteristics are reasonably well known.

The validation methodology adopted [117] involves blind predictions of selected hydrological responses, in which the modeller does not have sight of the measured catchment response data. The range of the predictions for each type of hydrological response is quantified based only on the catchment maps physical property data meteorological data and SHETRAN-UK simulations using any method provided it does not involve direct or indirect use of the measured catchment response data. These measured response data are retained by an independent referee and are released only after completion of the simulations and definition of the uncertainty bounds. The success of the prediction of each output variable is then checked by comparing the predicted bounds with the measured data.

Figure 5 Location of the Rimbauld Catchment



In the case of the Rimbaud validation, the work was undertaken before extensive experience of SHETRAN-UK had been obtained in post-closure radiological performance assessments. Thus, the uncertainty bounds were determined primarily by the researchers' beliefs in the compatibilities of the model rather than what might he required of it for assessment purposes. This led to the setting of narrow predicted bounds and a severe test of model performance.

For the SHETRAN-UK simulations the catchment was represented by a network of 144 grid squares of dimensions 100m x l00m with the channel network running along the boundaries of the grid squares (*Figure 6*). Data for the catchment were assembled during a two week field visit in June 1990. Time-series records of outlet discharge rainfall and other meteorological data were assembled for three three-year simulation periods: 1968-70 containing the biggest recorded flood) 1972-74 (a relatively wet period) and 1981-83 (a relatively dry period). The 1968-70 period was selected for use in the validation tests. Field and laboratory measurements included:

- Surface infiltration rates to derive estimates of the saturated conductivity for vertical flow;
- A permeability measurement to give an estimate

11 VALIDATION OF SHETRAN AT SLAPTON WOOD

The 0.94km^2 Slapton Wood catchment in south Devon was chosen to validate the SHETRAN-UK water flow component for the current UK climatic environment. The validation is one of three in which analogue catchments have been selected to represent the range of environments and climates which may characterise the catchments in the vicinity of the repository over the next few tens of thousands of years. Slapton Wood catchment is managed by the Slapton Ley Field Centre of the Field Studies Council and was chosen from a review of a number of possible UK lowland research catchments carried out by the Institute of Hydrology.

Catchment models are usually validated against the outlet discharge record only. Such a test indicates the ability of the model to reproduce the integrated catchment response in terms of observed streamflow, but does not indicate whether the simulated response is based on a sound representation of the internal catchment responses. A central element of the Slapton Wood validation was therefore to test the ability of SHETRAN-UK to simulate the internal catchment responses, particularly in the subsurface. To provide the necessary test data, the Institute of Hydrology installed an extensive set of equipment for monitoring soil moisture and phreatic surface levels, additional raingauges and an internal stream gauging structure. A drilling programme, soil survey and a survey of the channel network were carried out and time series data were collected for the period November 1989 - March 1991.

In order to test the predictive capability of SHETRAN-UK, a “blind” validation was performed in which the modellers were not allowed sight of the measured output data until the simulations were finished. in the method, upper and lower bounds are set on the values of the model parameters, reflecting uncertainty in the values. Simulations are carried out with the different parameter values, producing an envelope of outputs. The measured output is then released by an independent referee. The success of the validation is judged according to predefined criteria, usually a percentage for the containment of the measured output within the simulated envelope bounds. In this way the uncertainties in the predictions of each type of hydrological response are quantified. The combination of blind and internal validation make the Slapton Wood application probably the severest test ever applied to a catchment model.

Three groups of tests, corresponding to the data availability, were defined for the validation:

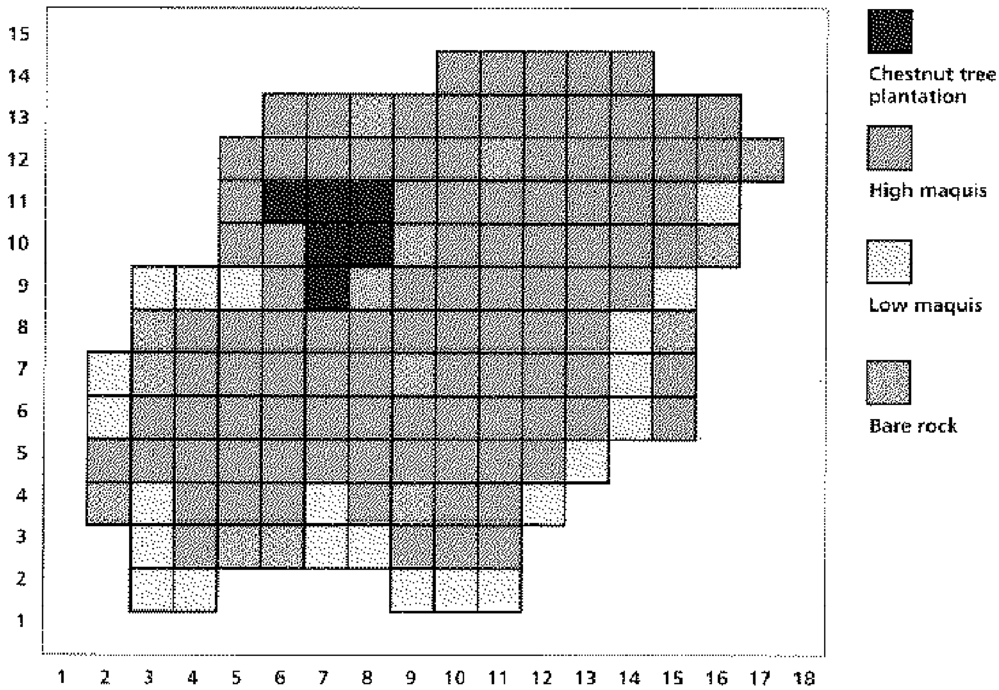
(1) Phreatic surface level at an internal location;

(2) Stream discharge at the internal and outlet gauging stations;

(3) Soil water (matric) potential at three internal locations

A two-stage validation was planned. In the first stage, output bounds were predicted “blind” for each test feature but only the measured phreatic surface level data were released for comparison. Depending on the results, the second stage might have involved calibration against the phreatic surface levels and a repetition of “blind” predictions for the stream discharges and soil water potentials. Results to date, though, indicate an excellent containment of the measured phreatic surface levels within the simulated bounds, probably the first time that such a result has been demonstrated for an integrated surface/subsurface catchment model. The second stage of the test, comparison of the measured stream discharges and soil water potentials, is now going ahead. Overall, the results so far justify the considerable thought and effort which have gone into the validation and generate confidence in the capabilities of SHETRAN-UK to simulate the behaviour of hypothetical future catchments.

Figure 6 Representation of the Rimbauld catchment for the simulation studies using SHETRAN-UK



of the saturated conductivity for lateral flow;

- Soil particle size distributions for prediction of hydraulic properties (see [118]);
- Soil profiles, soil depths and root zone depths.

Vegetation distributions were obtained from aerial photographs and a SPOT satellite image. Three main types were identified:

- A dense natural cover of grass, shrubs, maquis and trees covering much of the catchment;
- A cleared band with subtree vegetation along the road network;
- A chestnut plantation near the catchment outlet.

The measures selected for validation and the criteria for successful validation are summarised below. (The measures selected, the criteria and the predicted bounds were all specified by the modellers before the observed data were inspected.)

Results from Test A for 1968 are provided in Figure 7, which shows the predicted bounds, measured bounds and normalised index of success, I. In this figure, I is defined by:

$$I = (Q_{obs} - Q_{min}) / (Q_{max} - Q_{min})$$

where Q_{obs} is the observed discharged rate, Q_{min} is the minimum bound value and Q_{max} is the maximum bound value. Only the periods for which the maximum bound exceeded 25 $l\ s^{-1}$ are plotted.

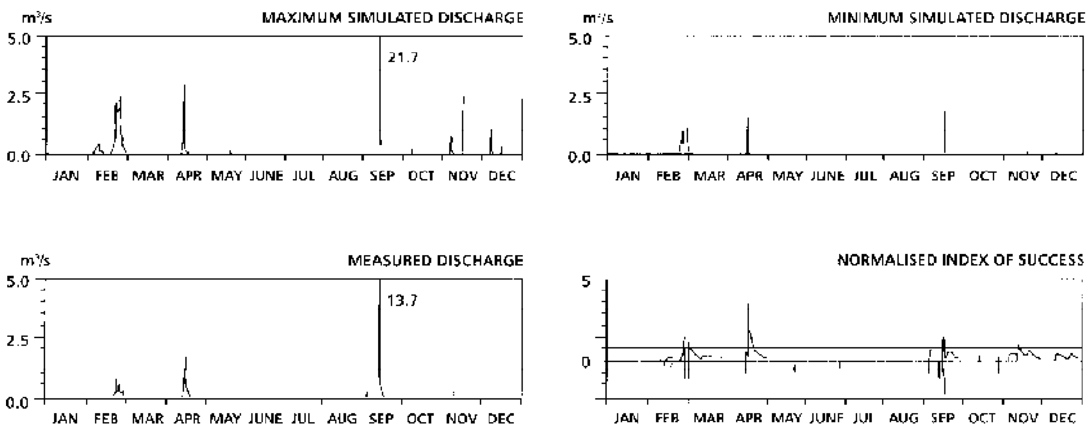
The observed discharge fell within the predicted bounds for 78% of the time. In general, the storm-discharge peaks were over-predicted, and storm runoff was less flashy than predicted. This resulted in the observed discharge data being outside the bounds for short periods around the storm peak, and for longer periods during the early part of the storm recession. This effect is thought to arise because the only mechanisms fear

	Description	Criteria for successful validation
Test A	Continuous discharge hydrograph (15 minute intervals) for 196-1970, for periods where the maximum predicted discharge rate exceeds 25 l s^{-1} (approximately the mean discharge rate over the three years).	The observed discharge rate must fall within the predicted bounds for at least 90% of the time.
Test B	Peak discharge rates for all clea4y identifiable storms where the maximum predicted discharge rate is greater than 0.5m^3 s^{-1}. For cases where more than one storm is predicted within any 24-hour period, only the storm with the highest peak discharge rate is included. (32 storms were identified during the three-year simulation period).	Observed peak discharge rates must fall within the predicted hounds for 28 out of the 32 storms (approximately 88% of the total). To allow for storms which are no)t predicted, the test will fail if more than 4 clearly identifiable storms occur where the peak discharge rate is greater than 0.5m^3 s^{-1}, which are not included in the set of predicted peaks. For cases where more than one observed storm occurs within any 24-hour period, only the storm with the highest peak discharge rate will he considered.
Test C	Total monthly runoff for each of the 36 months of 1968-1970, excluding any dry months where the predicted monthly mean discharge rate is less than 25 l s^{-1} (13 wet months were identified during the three-year period).	The observed total monthly runoff must fall within the predicted bounds for 11 out of the 13 months (approximately 85% of the total). To allow for wet months which are not predicted, the test will fail if more than 3 wet months occur in the measured data (mean discharge greater than 25 l s^{-1}) which are no)t included in predicted set of wet months.
Test D	Total runoff for the whole of the three-year period.	The observed total runoff for the three-year period must fall within the predicted bounds.

generating streamflow in this version of SHETRAN-UK are overland flow and saturated subsurface flow. This means that simulated hydrographs tend to be clearly delineated into a baseflow and a flashy surface runoff response. An intermediate, interflow response call be generated in the field through soils very close to the ground surface, or above discontinuities in the soil profile between layers with different hydraulic properties. These factors are likely to have been of significance at Rimbaud. A new Variably Saturated Subsurface (VSS) component of SHETRAN-UK is currently being implemented which will have the capability of simulating interflow effects (*see subsection 4.3)* .

The predicted bounds and measured peak discharge rates for Test B are shown in Figure 8. The measured data fall within the predicted bounds for 13 out of 32 storms, compared with 28 out of 32 required for success of the test. These results reflect the over-prediction of peak discharge rates described above. However, the capability of SHETRAN-UK to simulate storm responses of

Figure 7 **Validation of SHETRAN-UK for the Rimbauld catchment: Test A - continuous discharge hydrograph for 1968. For definition of the normalised index of success, see main text.**



greatly different magnitudes arising from different runoff mechanisms is clearly demonstrated.

In respect of Test C, the measured data fell within the predicted bounds for 10 out of the 13 months (*Figure 9*) and there were no unpredicted wet months. For Test D the observed runoff over the 36 month period was found to fall near the centre of the predicted bounds, indicating that the overall mass balance for the catchment was approximately correct.

Although only one out of the four tests passed the specified criterion, the Rimbaud validation study has given considerable confidence in the predictive capabilities of SHETRAN-UK, especially as this was the first validation test of this type that has been run for the SHETRAN-UK modelling system (or, as far as is known from the literature, for any other model). Specifically, the capability of SHETRAN-UK to simulate the interactions between surface and subsurface runoff for storms of greatly differing magnitude was demonstrated, while the aspects of the model that led to the over-predictions of storm peaks and the undue sharpness of the subsequent recessions were readily identified. It is of interest to note that the need for a new vss component of the model had been recognised before the results from the Rimbaud validation study became available.

It is also noted that the ease with which validation is achieved is strongly conditioned by the width of the bounds set. In this study, the validation team set tight bounds, based on their beliefs in model performance (*see Figures 8 and 9*) and the results achieved suggest that, even though these bounds were not satisfied, predictions of the discharge associated with individual storms and of monthly runoff can be made accurate to within a factor of two. With more extensive data on catchment characteristics, it seems likely that even more accurate predictions could be made.

Overall, the results from the Rimbaud validation study give substantial assurance that the results on water routing and contaminant transport being obtained from the hypothetical catchment studies (*subsection 4.4*) provide a physically realistic picture of what is likely to occur in such catchments. The demonstration that a blind validation methodology can be carried through for a physically realistic model is, in itself, an important advance, since it justifies the application of such a model to future hypothetical catchments [1].

4.2.2 Experimental Studies at the Intact Core and Field Plot Scales

The overall aim of the core and plot experiments is the derivation of datasets relevant to contaminant migration for use in internal-state validation of SHFTRAN-UK and parameter upscaling procedures [122, 123]. As emphasised by Beven [122], the data required as input to SHETRAN-UK are effective parameter values for hydraulic conductivity and moisture release, and transport parameters of dispersivity and mobile volume for every grid-element within the flow domain. Ideally, measurements of flow and transport parameters should he derived in field plots, which can be of dimensions comparable with those of a single grid element. However, in practice, the largest spatial scale that can be contemplated for regular use is that of intact 'undisturbed' soil cores, brought back to the laboratory. Studies on such cores have been included in the biosphere sector of the NSARP for several years *(see Box 12)*.

The validation experiments have centred on multiple tracer testing within two 30m square field plots. These experimental sites are located at the Hazelrigg field station, Lancaster University and at Calder Hollow, near Sellafield. Measurements of hydrometric and chemical data have been obtained following the injection of chemically conservative chloride, and reactive tracers including strontium, rhodamine WT and lanthanum (*see Box 13*). Intact cores have been

Figure 8 **Validation of SHETRAN-UK for the Rimbauld catchment: Test B - peak discharge rates during identified storms**

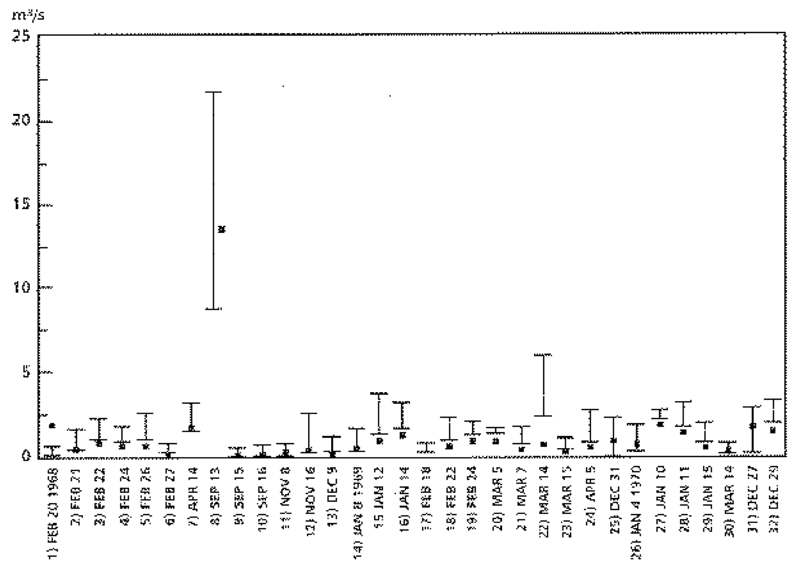
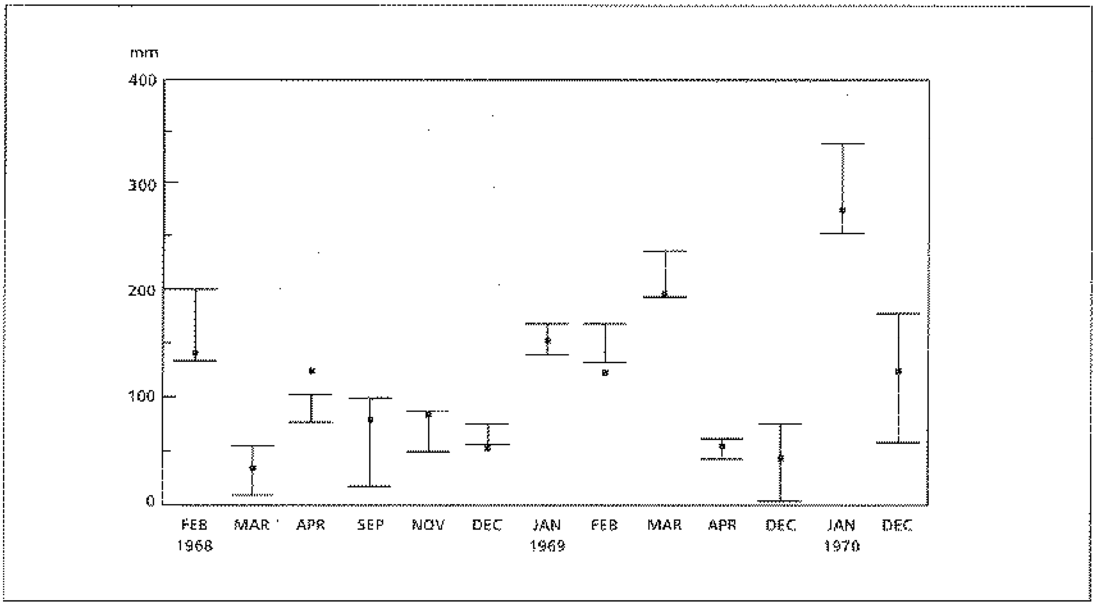


Figure 9 Validation of SHETRAN-UK for the Rimbauld catchment: Test C - monthly discharge during wet months



extracted from both sites and the transport parameters derived from breakthrough experiments.

The tracer tests at Hazelrigg were conducted within a cambic stagnogley developed on the deep tills of northern Lancashire. These materials are clay-rich and exhibit a marked decline in the saturated hydraulic conductivity (K_s, ms^{-1}) with depth (d, m) where $K_s = 1.056\ 10^{-7}\ d^{-2.5}$. A perched groundwater system is generated with a phreatic surface fluctuating by around ± 0.3m at about 0.3m depth. Furthermore the clay-rich nature of the soil promotes a wide distribution of pore-scale migration velocities. In other words the soil has high rates of preferential (macropore) flow and very slow losses of water from other pores. Within SHETRAN-UK, this is parameterised using the mobile-immobile extension to the advection dispersion equation (ADE). Testing at Hazelrigg therefore allows the SHETRAN-UK implementation of the extended ADE. to be validated.

Simulation of the chloride (Cl) tracer test at Hazelrigg (*see Plate 5a*) has been carried out. For simulation purposes the plot area is represented by 307 columns of varying plan area (from a minimum of 1m by lm to a maximum of 5m by 3.5m). Variable lateral grid spacing was employed for two reasons: so that a finer grid resolution could be achieved around the tracer source (where development of the plume would occur quickly) and to allow for the explicit inclusion of the subsurface tile drains at 0.7m. Each column has a vertical finite-difference cell spacing of 0.025m through most of the column length, reducing to 0.01m towards the top of the soil profile. The soil hydraulic properties were discretised into three layers. Successful simulation of the Cl breakthrough was achieved with SHETETAN-UK. Plate 5b shows the breakthrough at O.5m depth within the profile some 2.5m downslope of the line-source of tracer

12 CONTAMINANT TRANSPORT STUDIES IN INTACT CORES

A significant problem in making distributed predictions of the transport of contaminants in the near surface zone is the specification of appropriate model parameters for the advection-dispersion equation (ADE). The processes of flow through soil are very complex in detail, especially under near-saturated conditions or at high flow rates, when the effects of macropores due to cracks and root channels and other biotic influences may lead to marked and rapid preferential movements of contaminants. This has been demonstrated at Lancaster University in tracer experiments on large undisturbed soil cores *(Plate A).*

Experiments have been carried out for transport both by rainfall falling on the soil surface, and for tracer applied in water at the base of the column to mimic the return flow of water from deeper layers. Mixing of simultaneous rainfall and return flow inputs has also been studied using multiple tracers, which means that the contributions to the discharge from the column due to each source can be separated *(Figure A).* This work has concentrated on using relatively conservative tracers.

The ADE, as used in SHETRAN-UK, will usually describe the resulting tracer breakthrough curves successfully *(Figure B)*, with a modification to allow for the fact that only part of the water-filled pore space in the soil is effective in the rapid transport process. The simplest ADE model then has two parameters: a dispersivity and the proportion of the pore volume occupied by 'mobile' water.

Tracer experiments on large undisturbed soil cores are very time consuming and only a small number can be carried out. The presence of preferential flow, however, suggests that the dispersion process (and therefore the model parameters derived to represent it) will vary markedly with the particular structure of individual soil cores. Thus, it is difficult to scale these parameters up to the grid sizes typically used in a distributed model such as SHETRAN-UK. At that scale, effective parameter values are required that reflect the distribution of transport processes within a grid element.

A methodology has been developed at Lancaster to allow the information obtained from one or a small number of core experiments to be used to estimate these effective parameters. This methodology uses a Bayesian approach to derive a distribution of possible grid-scale parameter values conditioned on the available measurements and an assumed variance for the intra-grid variability.

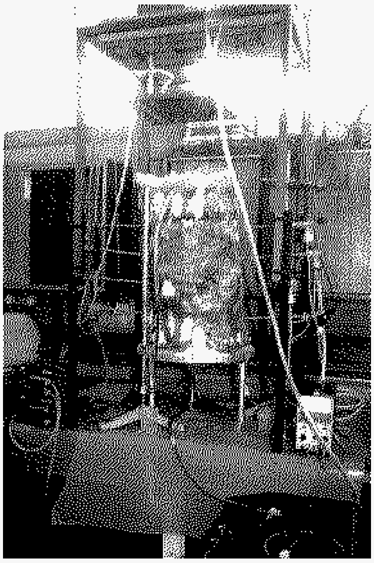


Plate A: A large intact core being studied in the laboratory

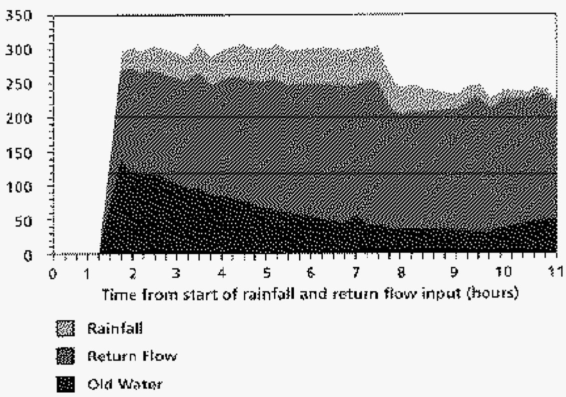


Figure A: Flow separation of tracer-labelled rainfall and return-flow (added to top and bottom of an undisturbed soil core, respectively), Rainfall was added only for the first 7 hours.

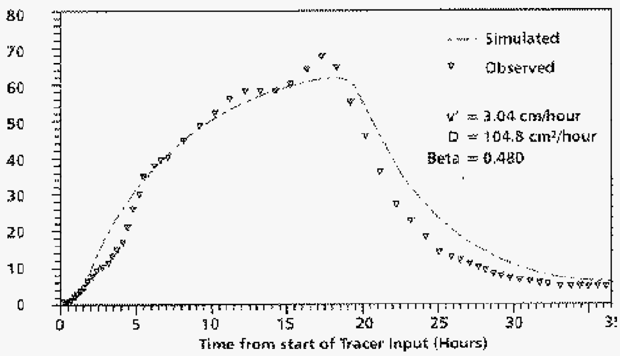


Figure B: Fitted breakthrough curve for return flow through a large undisturbed soil core. Note the very rapid initial breakthrough and long tail indicative of preferential flow in macropore pathways and a very high dispersion coefficient.

13 INSTRUMENTING FIELD PLOTS FOR CONTAMINANT MIGRATION STUDIES

The migration of water tracers has been monitored within two 30m square field plots. These experimental sites are located at the Hazelrigg field station, Lancaster University and at Calder Hollow, near Sellafield [Plate 6]. The hydrometric and chemical data monitored during multiple tracer tests are being used in the validation of SHETRAN-UK. For the Calder Hollow dataset, rigorous 'blind validation' will be applied.

The experiments at Hazelrigg were conducted within the upper O.7m of an under-drained cambic stagnogley. At Calder Hollow, tracers were injected into sand strata (at depths of 2 and 4m) within a 6m deep glacio-lacustrine drift. For the Hazelrigg tests, a sprinkler system was used to keep the soil moisture status high to reduce the system transients. In contrast, tracers were applied to the Calder Hollow drift under natural, dynamic moisture conditions.

Chemically conservative chloride (Cl) weakly reactive strontium (Sr) and rhodamine WT, and strongly reactive lanthanum (La) were used as tracers at Calder Hollow. The development of three-dimensional profiles of these tracers within the plot was studied using direct and analogue techniques. Spot samples of soil water were extracted from boreholes and vacuum samplers distributed throughout the plots, and then analysed for ion concentration within the laboratory. These data were interpolated temporally using datalogged measurements of fluid resistivity within the boreholes. Interborehole spatial interpolation was achieved with the aid of surface- and borehole- based measurements of ground resistivity. The plume development in plan after 13 days of chloride injection is shown in Plate 5a. These data are based on a twin-electrode survey of ground resistivity. The injector arrays are at 15E, 13N.

At both sites, the dynamics of moisture potential and volumetric moisture content within the upper layers of drift and solum were monitored using electronic tensiometers and neutron moderation. Borehole nests were used to monitor positive moisture potentials throughout the flow fields of both plots.

The hydraulic and transport properties of both plots were determined using in situ ring permeametry, recharge and recovery tests, moisture release, particlesize analysis and laboratory breakthrough experiments. The breakthrough experiments were conducted on undisturbed soil cores encased in either fibreglass or steel (see Box 12).

At Hazelrigg, the Cl plume migration and dilution by rain-water was monitored over a 10 month period. In contrast, shorter duration, 11 to 39 day, experiments were conducted at Calder Hollow. The chloride and strontium tracers administered at Calder Hollow were observed over migration distances of up to 20m.

input. Storm-based distribution of the tracer plume by rainwaters is observable around the peak of the breakthrough curve shown in plate 5b.

In contrast to the tracer tests conducted at Hazelrigg, those carried out at Calder Hollow, near Sellafield were within the sand strata of a 6m deep glacio-lacustrine drift (*Plate 6*). This glacially overridden deposit characterises most of the surrounding lower Calder/New Mills catchment. Marked field-scale anisotrophy in the saturated hydraulic conductivity, as measured in recovery and slug tests [124, 125, 126] is observable within the drift, with the sand layers having conductivities ranging from 10^{-4} to 10^{-6} ms^{-1} and the interbedded clay-rich layers only 10^{-8} m s^{-1}. A pronounced NW-SE dip in the drift stratigraphy is apparent. Plate 7, for example, shows coarser layers closer to the ground surface (*ie* high ground resistivity) in the NW corner of the 30m experimental plot.

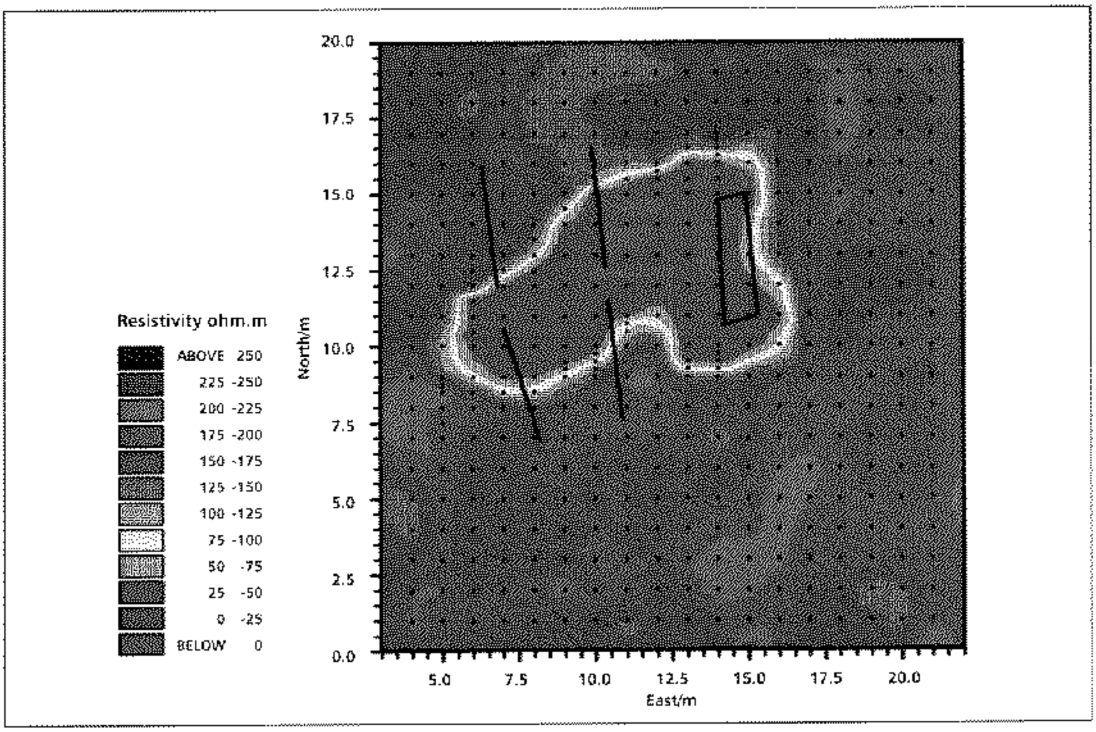
Migration of both chloride and strontium was rapid and remained largely within the sand layers receiving the injected tracer. As at Hazelrigg, development of the three-dimensional tracer plume was studied using direct and analogue techniques (*see Box 13*). Spot samples of soil water were extracted from boreholes and then analysed directly for ion concentrations. These data were interpolated temporally using datalogged measurements of fluid resistivity, and interpolated spatially with the aid of ground-resistivity measurements.

Validation of the SHETRAN-US simulation using the Calder Hollow data, will take place using a 'blind validation' strategy, as with the studies at Rimbaud. Results of the plume development cannot be released until the associated blind validation simulations are complete.

4.3 Future Developments of the Model

Although the current version of SHETRAN-UK

Plate 5a: Tracer distribution in plan within the Hazelrigg field plot. This visualisation was made after 13 days of chloride injection, and is based on a twin-electrode survey of ground resistivity.



provides an extremely useful tool for exploring water flow and radionuclide migration in a wide range of different catchment types, there are three areas in which developments of, or extensions to, the system have been identified as desirable. These are:

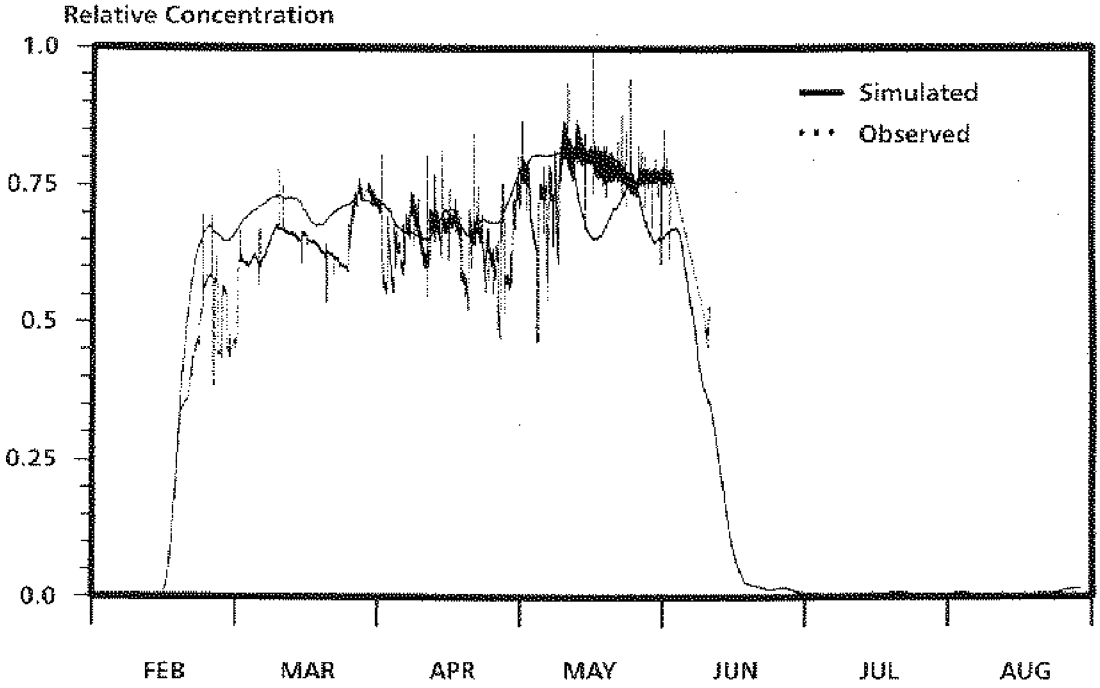
- Replacement of the subsurface flow components of the model with a new variably saturated component to represent more adequately areas of complex lithology;
- Incorporation of a cold-region component into the model to represent frozen-ground effects;
- Extension of the timescale of modelling from decades to centuries.

Progress in each of these areas is outlined below.

4.3.1 Enhancement of the Variably Saturated Subsurface Component of the Model

The subsurface is currently represented within SHETRAN-UK by three components: the saturated zone component, which uses the vertically averaged Boussinesq equation to simulate 2-D flow in unconfined aquifers only; the unsaturated zone component, which uses Richards' equation to simulate vertical flow in the unsaturated zone above the water table, and is coupled to the saturated zone solution by a mass-balance procedure; and the aquifer-channel exchange component. These three components are being replaced by a new Variably Saturated Subsurface (VSS) component, for which a descriptive functional specification is outlined below:

Plate 5a: Hazelrigg plot experiments: Measured and simulated breakthrough curves at a depth of 0.5m within the soil and 4m downslope of the chloride source



- Fully 3-D flow in single porosity/single permeability porous media is simulated; flow through fractured media can be represented for conditions where an equivalent porous medium model is appropriate;
- Flow through multiple layers of porous media of different characteristics can be simulated; the layers can be laterally extensive, discontinuous, or of limited lateral extent;
- Confined, semi-confined and unconfined aquifers can be represented;
- Groundwater perching above low permeability lenses can be represented;
- The lower boundary condition is either a prescribed, time-varying water flux into the model domain or a free-drainage flux out of the model domain;
- The edge boundary conditions are either a prescribed, time-varying head or a prescribed time-varying water flow for each layer;
- The upper boundary conditions are either a prescribed, time-varying head, when ponded surface water is present, or a mixed-type, when no surface water is present, and there is precipitation/evaporation at the ground surface; switching between these two types of boundary condition is automatic.

With this enhanced subsurface flow model, extension of the transport component to accommodate lateral migration in the unsaturated zone is a minor modification to the existing component.

14

THE UP MACROMODEL AND SOME OF ITS APPLICATIONS

The UP (terrestrial hydrology) macromodel is one component of a distributed, physically based, large-scale modelling system which contains a hierarchy of coupled terrestrial hydrology and atmosphere models at scales ranging from 100m to 50km. The system was designed primarily to allow the study of the impact of changes in climate and land-use, with the flexibility to follow impacts from scale to scale. UP, the name, is derived from 'upscaled physically based' and the UP macromodel can be viewed as an extension of physically based, SHETRANUK type, modelling (Box 10) to larger scales and long-term simulation. The large-scale modelling system (which does not yet have a name) is being developed as part of the work of several research projects involving regional climate modelling, (continental scale) hydrological modelling in the Mississippi basin, and large scale desertification studies in Spain and Portugal. Only the UP macromodel is discussed here, as only the terrestrial hydrology components of the full system are being used in work for UK Nirex Limited.

When using the UP macromodel, the area being modelled is divided into sub-catchments, each containing a single stretch of main channel. Combined, the stretches of main channel form a coherent drainage network linking together the sub-catchments (which may also be linked by regional groundwater flow pathways). Flow in the network is modelled using the diffusion form of the Saint Venant equations, the individual sub-catchments being modelled as four-compartment storage elements (Figure A).

Two of the key features of the UP macromodel are the large size of the sub-catchments, and the simplicity of the parameterisations of the four-compartment storage elements (Table A). These features allow the UP macromodel to run very quickly; one hundred times faster than SHETRAN-UK. What is equally important, though, is the way in which the parameterisation is carried out. Research has led to a new method which gives good parameterisations (always difficult to achieve when upscaling) and allows time-varying 3-dimensional fine-scale storage and flow fields to be created based on simulation results from the UP macromodel. These fine-scale fields are consistent with the macromodel results, and can be used in fine-scale impact simulations, allowing impacts to be followed from the UP scale to the fine scale.

The new method for parameterisation involves using fully detailed fine-scale data sets for physical properties, topography, etc. (eg data on a 500m or 1 km grid). These are used in fine-scale distributed, physically-based simulations run using a suite of models created specially for this purpose. The UP parameterisation for a given sub-catch ment is in effect an accurate summary of the fine-scale flow and storage conditions for sets of (numbered) fixed hydrological states.

Fast running sediment and solute transport models have been developed to allow the simulation of impacts at the fine scale. These are based on the sediment and solute transport capabilities of SHETRAN-UK (Box 10), and use a combination of particle tracking and finitedifference algorithms. If time series data for the simulation variables for a sub-catchment are saved during an UP macromodel run, these can be used to create time series for state numbers. Based on these, 3-dimensional fields can be recovered and used to drive sediment and solute impact simulations. In this way, a century long simulation of radionuclide migration from a buried source can be run for a typical catchment in an hour on a standard computer workstation.

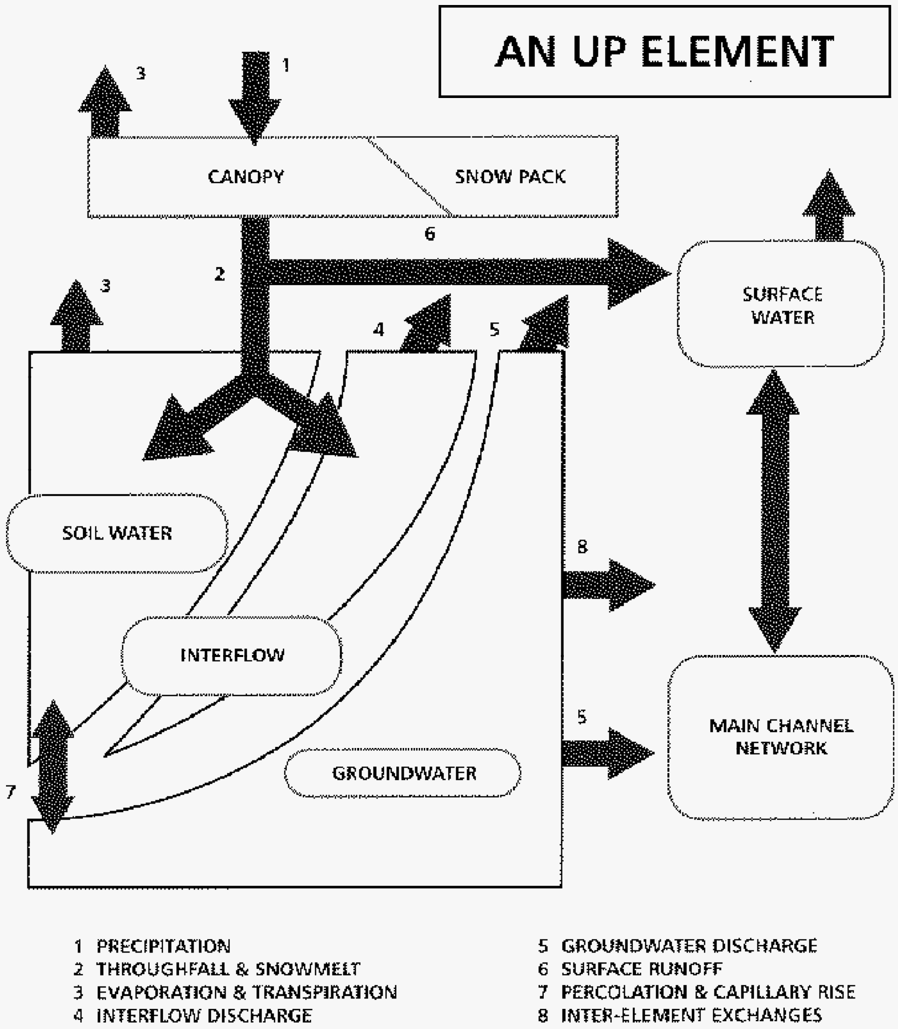
4.3.2 Incorporation of a Cold Region Component

It was recognised at an early stage of SHETRAN-LIK development that modelling of periglacial and colder boreal conditions should take account of those hydrological processes specific to cold regions. However, it was also considered that this topic was best addressed after some experience had been gained in running the first generation model and that implementation of a cold region component would probably require access to the facilities available in the new VSS component. For this reason, work to date has been limited to a review of cold region processes and possible approaches to their simulation.

In this review, attention is being concentrated on three main areas:

- The effects of soil freezing on runoff generation and subsurface flow;
- Groundwater discharge, stream-aquifer interactions and channel processes in cold regions;

14 THE UP MACROMODEL AND SOME OF ITS APPLICATIONS



- Snow accumulation and melting.

In addition, some attention is being given to the secondary, direct effects of low temperatures on contaminant behaviour (*eg* solute rejection during freezing).

To date, substantial progress has been made mainly in drawing up a specification for a heat transfer model that can be used to simulate freezing and thawing in the surface and near-surface. Because the partial differential equations governing heat transfer are very similar to those for contaminant migration, it is possible to adapt the existing SHETRAN-UK contaminant transport model to simulate heat transfer with freezing and thawing. However, this adaptation would require a substantial modification to the existing system to include feedbacks from the heat transfer model to the water flow model. In contrast, in the current version of SHETRAN-UK, information is passed from the water-flow component to the contaminant transport component, but not in the reverse direction.

In surface waters, it is thought appropriate to assume that all freezing and thawing takes place at 0°C. In the first instance, surface ice (whether in channels or at the ground surface) may simply be treated as a sink or source to which liquid water-is lost on freezing, and from which water is released on thawing. The feasibility of incorporating other effects of surface or channel ice accumulation in the model is an on-going topic of investigation.

In the subsurface, water held in porous materials tends to freeze and thaw over a range of temperatures, rather than at one particular freezing point. This is because capillary and adsorptive forces holding water within the pore systems of soils or aquifer materials must be overcome in order for freezing to progress. Some soil moisture may, therefore, remain in a liquid, mobile state even below the (normal) freezing temperature for bulk water at atmospheric pressure. The progressive reduction of liquid soil moisture content through transformation to ice during freezing brings about corresponding reductions in matric potential and hydraulic conductivity in much the same way as drying in unfrozen soils. It is, therefore, proposed that the effect of freezing and thawing on the liquid moisture status of a soil may be modelled by analogy with the wetting and drying processes in unfrozen soils. In this approach, it would be assumed that similar relationships to those for unsaturated unfrozen soils can be used to relate liquid soil moisture content to matric potential and hydraulic conductivity in freezing soils. This approach has been employed in several previous modelling studies of freezing in soils [127 - 131].

The only additional relationship needed is one which relates the heat state of the soil to its moisture state during freezing. Following the approach outlined in Williams and Smith [132], it is proposed that the unfrozen liquid water present with ice in a freezing soil be taken to have a matric potential that is independent of soil type, but depends on temperature through the Clausius-Clapeyron equation [133]. This approach can be used both to calculate the freezing point depression (and, therefore, the temperature at which the water-ice phase change commences) and also to derive the matric potential during such a phase change and hence the liquid moisture content, ice content and hydraulic conductivity.

In order to confirm the viability of this approach, the effects of freezing on soil hydraulic properties have been demonstrated in a preliminary application of the Clausius-Clapeyron relationship in the development version of the VSS component of SHETRAN-UK. In respect of boundary conditions for the heat transport model, the bottom boundary can be held at a fixed temperature, whereas at the top boundary a dynamic boundary condition would be required. This would entail a calculation of the energy budget at the ground surface, and would require upgrading the SHETRAN-UK vegetation canopy and snowpack models to include a representation of their heat transfer properties.

4.3.3 Extension of the Timescale of Modelling

Typically, SHETRAN-UK is used to simulate the properties of moderately sized catchments (a few tens of square kilometres in area) over timescales of up to about 30 years. Such a timescale is appropriate to poorly sorbed contaminants in such catchments [1] but is short compared with the timescale for transport of highly sorbed contaminants and with the overall assessment timescale. For this reason, there is a requirement to develop a general purpose macromodel capable of predicting flow and transport for larger areas and longer time spans than can SHETRAN-UK.

Work on this macromodel, the UP model (*see Box 14*), is funded jointly by UK Nirex Ltd, the Natural Environment Research Council (under the TIGER Programme) and the European Commission (under the MEDALUS Programme).

The water-flow component of the macromodel comprises a land-surface (runoff generation) module and a routing module. The routing module, which has been completed, is based on a

transfer function solution to the linear-parabolic convection-diffusion approximation to the Saint Venant equation. The land-surface module is currently under development. In overall terms, the modelled area is divided into drainage areas and runoff generation in each such area is estimated using a land-surface model, which is parameterised using aggregated results obtained running fine-detailed flow models. Areas in which work is on-going in the context of the land-surface model relate to the vegetation canopy, flooding, evaporation, snowpack, soil-moisture storage, interflow and groundwater modelling.

Work on the contaminant transport component of the macromodel is at a relatively early stage, but a combination of particle tracking and finite-difference techniques has been demonstrated successfully.

4.4 Status of the Research, and Its Relationship to Assessments and to Site Characterisation

For the last two years, a production version of SHETRAN-UK has been available for application in assessment studies and in site characterisation. Over that period, extensive use of the model has not revealed any significant deficiencies in performance relative to specification and considerable experience has been obtained in applying it in a wide variety of contexts. The recognised limitation of the water flow component of the model has been addressed by developing and implementing the new vss component, and the possible inclusion of cold-region processes in the model has been addressed through a comprehensive review. Validation of the water flow component of the model has made substantial strides forward, notably with the completion of the blind validation exercise for the Rimbaud catchment. In the context of validation of the contaminant transport component milestones have been the successful completion of the field plot experiments at Hazelrigg and the commencement of a similar, but more extensive, set of field plot studies at Calder Hollow, Sellafield. Already, these site-specific studies are starting to yield useful results for the further validation of SHETRAN-UK.

Also of considerable importance are the developments in macroscale modelling. The macroscale model is very closely related to SHFTRAN-UK, so that detailed comparisons of the results obtained from the two approaches can be made. Initial indications are that the macromodel will run at least one hundred times faster than SHETRAN-UK, so that simulation periods of more than one thousand years can be adopted and detailed sensitivity studies can be undertaken. Overall it is clear that SHETRAN-UK is the most comprehensive model available worldwide for simulating near-surface hydrological processes sediment transport and contaminant migration. This is evidenced by the degree to which on-going developments of both SHETRAN-UK and the macromodel are being funded by organisations other than UK Nirex Ltd.

Finally it is appropriate to note that SHETKAN-UK Is being used directly for assessment purposes. By 1992 it had been recognised that the release to the biosphere of poorly sorbed radionuclides such as ^{36}Cl and ^{129}I was likely to be of significance in any post-closure radiological performance assessment. Quantitative studies further indicated that the peak individual risk from such radionuclides was likely to occur in the first few thousands to tens of thousands of years after repository closure. Over this period temperate and then boreal conditions are expected to prevail in the British Isles. For this reason, it was decided that SHETLTAN-UK should be used to explore the distribution and transport of poorly sorbed radionuclides in hypothetical catchments judged to be characteristic of future temperate and boreal conditions. Furthermore because discharge to a terrestrial environment was judged more likely to occur in the reduced sea-level conditions characteristic of a boreal period the hypothetical boreal catchment was given priority. Thus, simulations of the distribution and transport of conservative tracers ^{36}Cl and ^{129}I in a hypothetical boreal catchment have recently been completed [1] whereas those for a hypothetical temperate catchment are scheduled to be completed by April 1995.

The temperate catchment is described as hypothetical because it is based on conditions in the Sellafield area at the present day supplemented

Plate 6: The Calder Hollow field site

15 NEAR-SURFACE HYDROLOGICAL STUDIES BEING UNDERTAKEN IN THE SELLAFIELD AREA

A number of “Near Surface Hydrological Study” contracts are being undertaken for Nirex, many of which have considerable relevance to the Biosphere Research Programme. The current status of key projects is summarised below.

RIVERFLOW GAUGING STATIONS

In addition to the National River Authority (NRA) gauge on the River Calder at Calder Hall, gauges have been established on the Kirk Beck arid Black Beck and operated since March 1994. Work is currently ongoing to establish a gauge on the River Calder at Thornholme and its commissioning is anticipated in early June 1995. Selected data from the NRA gauges are also being recorded on an on-going basis.

HYDROMETEOROLOGICAL STATIONS

Six purpose-built meteorological stations have been established, predominantly at high altitude, to investigate hydrometeorological regimes in the study area. All stations comprise rainfall monitoring and two also incorporate full climate monitoring. The commissioning of these stations was staggered and occurred over the period July to September 1994.

GROUNDWATER

The NRA Sandstone water level monitoring network has been supplemented with a number of continuously recording gauges. Data sets are maintained for all NRA boreholes. Mine abstraction records have been acquired, and mine water levels are now monitored.

SOIL INVESTIGATION NETWORK

Seven soil investigation sites have been identified within the study area. At each of these sites, the intention is to determine:

- soil type and character
- soil hydraulic properties
- soil tensiometry

These sites will be established in February 1995 and a nine month investigation programme is scheduled. The range and period of monitoring may be extended at some sites following further review by the Biosphere Research and Site Characterisation Teams.

QUATERNARY BOREHOLE INVESTIGATIONS

The scope of works includes single boreholes at thirteen locations to define hydrogeology and geology. At approximately six of these boreholes, piezometers will also be installed into the Sandstone rockhead. Drilling works are scheduled to commence at the end of June 1995.

VARIABLE SECTION VARIABLE DENSITY (VSVD) MODELLING

This work entails modelling three representative hydrogeological sections of the study area as characterised by deep borehole investigations and using the finite element SUTRA model to determine to what extent groundwater flows are influenced by thermal effects and salinity distributions.

SURFACE HYDROGEOLOGICAL MODELLING

This programme of work comprises water balance and modelling phases. The water balance phase will be completed in mid-May 1995 and involves updating previous effective rainfall and recharge estimates for the study area in the light of new data from the riverflow gauging and hydrometeorological networks. The modelling work entails development of a preliminary dynamic groundwater model for the Sandstone in the study area using MODFLOW. This work will commence in mid-May 1995 and reporting is anticipated late in July 1995. This component of the work will also make use of data being acquired on groundwater levels for the Sandstone and riverflows for the Calder.

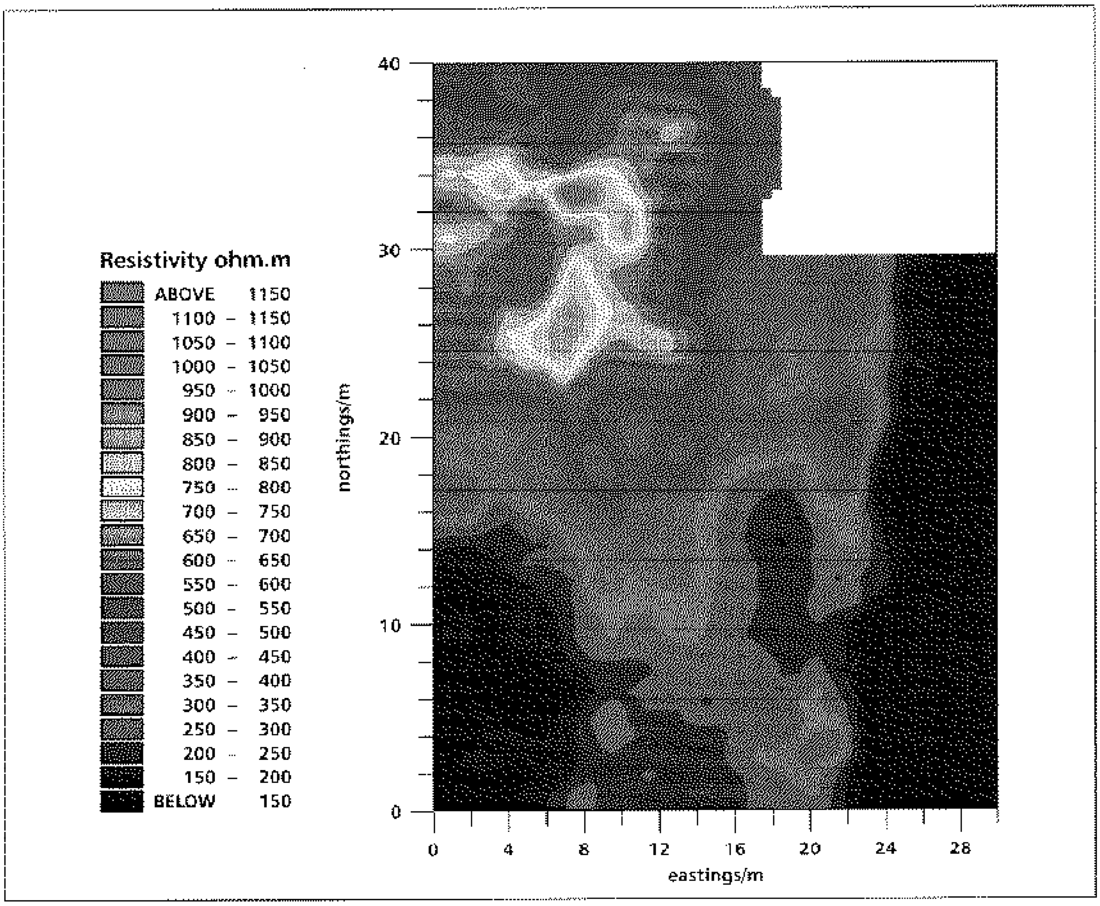
HYDROGEOLOGICAL MAP

An initial hydrological map for the study area has been completed. The map incorporates extracts from the geological and hydrological investigations described above.

by generic data, and making use of various geometrical and structural simplifications. As further near-surface geological and hydrological data arise from the Site Characterisation programme, this model will be refined until it can be described as a near-surface hydrological model of the site at the present day. Variants of this model will then be used to represent potential future temperate catchments in the vicinity of the site.

In moving towards such a site-specific model, significant inputs will come from the Quaternary characterisation programme *(see subsection 3.5 and Box 9)* and specifically from the near-surface hydrological programme *(Box 15)*, which includes studies on the hydraulic properties of soils and drift, surface water monitoring and meteorological monitoring. As this programme is already largely in place, a comprehensive, site-specific, near surface hydrological model can be expected to be developed over the next few years.

Plate 7: Ground resistivity survey, in plan, of the 30m square Calder Hollow plot and the site characterisation area to the northwest of the plot



5 Quantifying Radionuclide Transport in Soils and Uptake by Plants

As was noted in the previous review of the biosphere sector of the NSARP [4] a key area of uncertainty in catchment-scale modelling is the transport of radionuclides in the soil zone when contamination is from below ie in contaminated groundwater. More recent studies have emphasised this and have highlighted the particular importance of ^{36}Cl transfers in the soils and plants characteristic of cattle pastures. In view of these considerations since l988 the NSARP has included a programme of experimental studies on radionuclide transport in large soil-filled vegetated lysimeters complemented by detailed modelling studies. The objectives of this programme are to:

- Determine and investigate the key processes governing radionuclide distribution and transport in soils and uptake by plants;
- Determine parameter values characterising these processes for radionuclides of particular importance in assessments.

5.1 Status of the Research in 1992

Phase 1 of the experimental programme was well advanced at the time of the last review [4]. In the Phase 1 experiments a previously existing lysimeter installation at Silwood Park Ascot Berkshire was refurbished for use investigating the processes of radionuclide migration above near-surface (0.35m and 0.65m deep) water tables in a well-mixed soil and in studies of the partitioning of radionuclides in this zone between the soil and vegetation. Details of the construction and operation of these Phase 1 lysimeters is provided in Box 16 and a general view of them in operation is given in Plate 5.

The Phase 1 experiments commenced with a part season of radiochemical results in 1989 when ^{131}I was the only radionuclide used. In 1990 the first full experimental season was completed with the harvest of the winter wheat crop in July of that year. For this first full season the lysimeters were dosed with ^{137}Cs, ^{60}Co, ^{109}Cd, ^{22}Na, ^{99}Tc and ^{36}Cl in the spring and redosed on several occasions during the summer to maintain concentrations in the water table supply system (*see Box 16*). The unusually dry weather during that summer provided favourable conditions for radionuclide movement up the soil profile [4].

A second full season was completed in August 1991 with the harvest of the winter wheat crop. For this second season the lysimeters had been redosed in the spring with ^{60}Co, ^{109}Cd, ^{22}Na, ^{99}Tc and ^{36}Cl to replace radionuclides lost from the system in the winter months, mainly in the form of excess rainwater. No additional ^{137}Cs was added to the system in 1991 as analyses of soil cores taken prior to redosing indicated that little or no ^{137}Cs had been lost from the soil profile [4].

Overall the results of the experiments that were available by early 1992 indicated a strong dependence on climatic conditions and suggested significant differences in soil-plant transfer factors from those obtained in previous studies based on downward migration [4]

Modelling studies that had been completed by early 1992 comprised the development of a comprehensive fully coupled, soil-plant-water model [134] complemented with a solute transport model which was then used in all initial series of sensitivity studies [135] to provide guidance for future work (*see also Box 17 for a description of these models).*

Other modelling studies that were on-going in 1992 are described below (*subsection. 5.2*) but it is relevant to note that these various experimental and modelling studies were complemented by a series of process-oriented review studies relating to radionuclide transport at the catchment scale or within the soil zone. Thus by 1992 literature had been reviewed concerning:

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THE PHASE 1 LYSIMETER INSTALLATION

The objective in developing the lysimeter facility was to achieve as close to field conditions as possible, using natural soil and ambient hydrological inputs and outputs, with a winter wheat crop to be grown on the soil with reasonable root penetration and density, but with the constraint of the water-table being controlled at a specified level.

The eight concrete lysimeters, each approx. 2m x 1 m x 1 m deep, were sealed with rubber chloride paint, and provided with a substrate of polyethylene beads, a PVC manifold within the substrate, and a geotextile filter at the bead/soil interface. Construction materials were selected for low radiochemical sorptivity and provision was made to dose the water within the substrate with a radiochemical cocktail.

The lysimeters are intensively monitored. The following instruments are used (to measure the associated variable): tensiometers coupled to transducers (soil moisture suction), thermistors (soil temperature), floats coupled to potentiometers (water level in each buffer tank), probes for a Time Domain Reflectometer (soil moisture content), access tubes for a Neutron Probe (soil moisture content, again) perspex tubes for a borescope (root growth), an inclined point quadrat (leaf area index), platinum electrodes (redox potential). Most of these measurements are recorded in a programmable data-logger, and off-loaded to a PC computer at weekly intervals for inspection and archive; other data are measured manually and transferred to the PC archive.

Strictly, the water-table level in any soil is somewhat ill-defined. To overcome this, the design included a small external tank, directly connected to the Lysimeter substrate; the water level in this tank is held constant, and acts as a stabiliser or buffer for the water-table level in the Lysimeter. This buffer tank is connected via a peristatic pump to a large reservoir, common to all the Lysimeters, which acts as a source or sink of radioactive solution*(Figure A).*

The water level in the buffer tank is sensed by opto-electronic devices, which act as on/off switches depending on whether they are covered by water or not. Signals from these devices are fed to the data-logger, which, being programmable and having output ports, is able to control the peristaltic pumps and maintain the water level. When the sensor detects a falling water level, the pump moves water from the reservoir to the buffer tank, and, when the level rises, from the buffer tank to the reservoir. The water balance is measured by counting the revolutions in both directions of the pump, using a shaft-encoder plus decoding electronics.

Measurements from the various instruments are recorded at intervals of 1/1 00th of a day, and the resulting datafiles are timestamped with the year and the Julian Day (ordinal day in year); thus any timestep is defined uniquely by a single floating point number.

Manual measurements of soil moisture content are taken at weekly intervals. Samples of the radioactive solution, and cores drilled from the lysimeters, are taken at regular intervals for laboratory analysis.

In addition, an automatic weather station is located nearby to record relevant meteorological data.

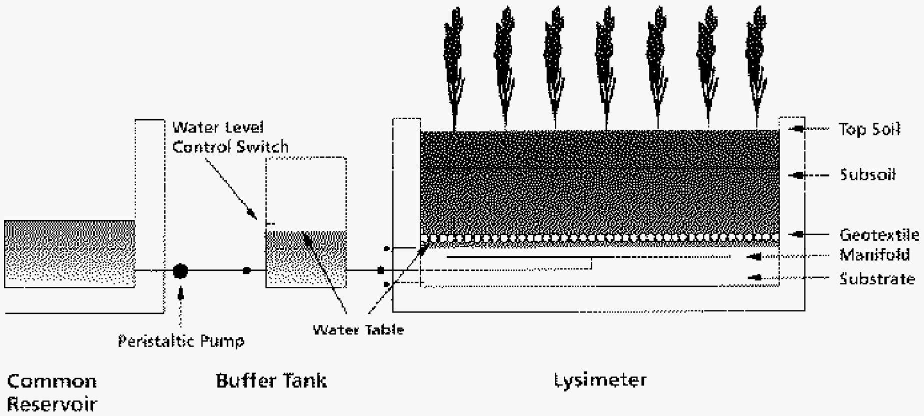

Figure A: Water level control in the phase 1 lysimeters (not to scale).

Plate B: The Phase 1 lysimeters in operation

- Biotic transport of radionuclides as a result of mass movement of soil by burrowing animals [136];
- Biotic transport of radionuclides in soils as a result of the actions of deep-rooted plant species [l37];
- Long-term retention mechanisms in soil which may affect losses from surface soils by erosion and resuspension with particular reference to watershed-scale transfers [138];
- Decomposition of organic matter and the modelling approaches used to describe the process [139];
- Volatilisation of radionuclides with particular reference to tin and iodine losses from soils and plants [140]; and
- Interception retention, absorption, and translocation of radionuclides by vegetation following application in irrigation waters [141].

In 1992 it was envisaged that four full seasons of data would be collected from the lysimeters and that analysis and interpretation of these data might require significant modificatios to the 1-D models already developed [4].

5.2 Experimental Studies Since 1992

As projected in 1992 [4] four full seasons of data were obtained from the Phase l lysimeters running in their original mode of operation. Thus the fourth winter wheat crop was harvested in August 1993. By this time it had been decided that the end of the useful life of these lysimeters was approaching and a plan had been prepared to use the fifth and final year of the experiment to explore some of the questions raised by the project that it had not been

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MODELLING WATER FLOWS AND RADIOCHEMICAL TRANSPORT IN SOIL-PLANT SYSTEMS

The uptake of radionuclides by plants from a contaminated groundwater source is governed by a variety of physical, chemical and biological processes. These control the transport of radiochemicals up through the unsaturated sotl profile and into the plant rooting zone, and the transport of the radiochemicals across the root epidermis and into the cortex tissue. Once within a plant, activity can remain stored in the root tissue, or undergo translocation up through the root system and into the above-ground components of the plant.

The interpretation of the experimental data being collected from the lysimeter facility *(see Box 16)* and application of those data in post-closure safety assessments is being undertaken through the use of modelling techniques. A simplified model of the entire lysimeter experiment, which simulates radiochemical concentrations in each component of the system, has been developed and provides a methodology for data assessment and quality control. It also provides a basis for more detailed, physically based models, which seek to incorporate the key processes affecting radionuclide behaviour within the lysimeters.

A hydrological model representing the movement and storage of soil water has been developed. The model, based on the Darcy-Richards equation, is driven by meteorological data, which provide the rainfall and evapotranspiration moisture fluxes, and is characterised by observed soil hydraulic properties. The output is used to drive a contaminant transport model which simulates the movement of radionuclides in the soil. This model incorporates the effects of advection due to bulk water motion, molecular diffusion, and dispersion, which arises from differential water flow velocities and matrix tortuosity. Physical entrapment and chemical sorption of the radionuclides by the soil matrix are also incorporated into the model's structure.

For plant uptake to occur, there must be a zone where contaminated soil overlaps the rooting profile *(see Figure A)*. Modelling soil-to-plant transfer, therefore, involves interfacing the results of the contaminant migration model with a plant-root uptake model. For annual crops, such as the winter wheat grown in the lysimeters, the overlap of the root system with the zone of soil contamination is a dynamic feature. Because pre-existing experimental data had shown that solute uptake by plant roots can be represented by Michaelis-Menten rate kinetics, this approach was adopted in the initial version of the model. In addition, experimental results from the lysimeters have pointed to the importance of chemical recycling by the plant system. Therefore, using information being derived from supplementary small-scale column experiments, these processes are now being incorporated into the models structure.

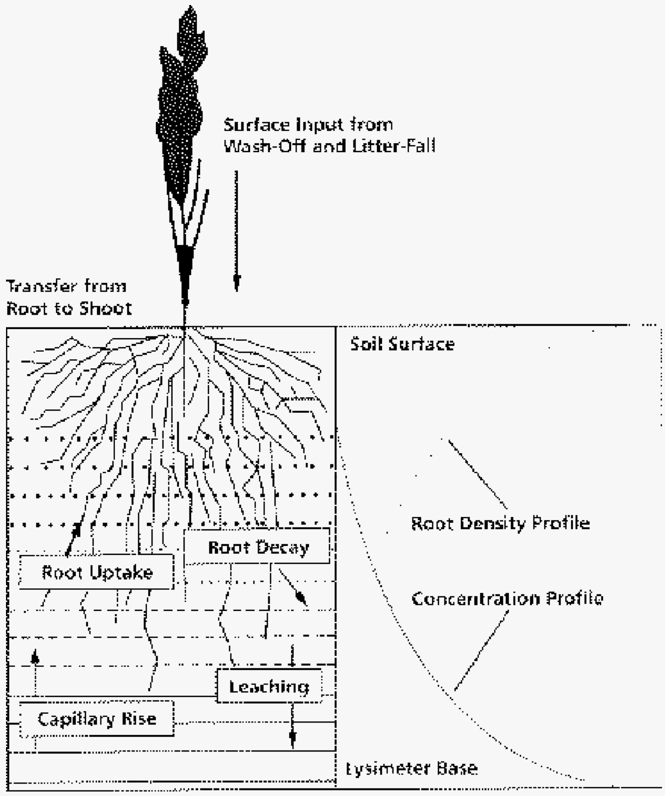


Figure A: Conceptualisation of soil-to-plant transfer processes

possible to investigate in the original mode of operation. This plan, which has now been carried out, involved applying different treatments to the eight lysimeters. Specifically:

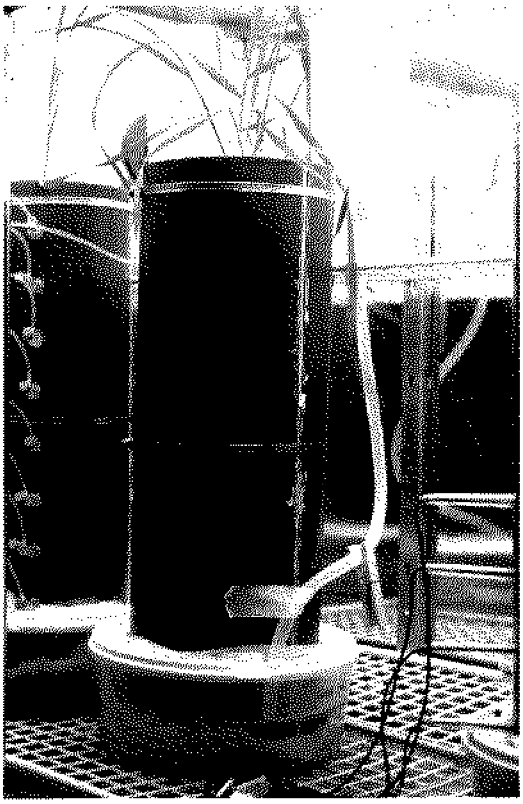
- To simulate the dry summer conditions of 1990, which were associated with enhanced soil-to-crop radionuclide transfers, rainfall input to two of the lysimeters was artificially restricted over the spring and summer of 1994;
- The effect of having a seasonal variation in the water table has been examined, in one lysimeter with a standard water table depth of 0.65m, by slowly raising the water table over the winter period to a depth of O.35m and then reducing it to a depth of 0.65m over the early part of the spring;
- In one lysimeter; the temporal dynamics of uptake into the wheat crop has been studied by destructive sampling at 21 times during the growing season, with each sampling involving the removal of 20 plants and one soil core;
- Two lysimeters have continued in the original mode of operation to provide control data for comparative purposes;
- Two lysimeters have been subject to destructive analysis, which has included the removal of a large number of soil cores for gamma analysis, determination of ammonium and Fe II / Fe III, determination of pH, and extraction of soil water for separate gamma analysis; in addition, the remaining soil, geotextile membrane and polythene substrate are being sampled from one lysimeter to allow an overall radionuclide budget to be made.

All the hydrological and radiochemical data from the first four full seasons have been stored on a database for subsequent analysis, and results from the variant studies undertaken in the fifth season will also be stored on this database.

In order to study radionuclide transport processes in more detail than is possible in the fullscale lysimeter experiment, a series of column studies have attempted to reproduce the lysimeter system in microcosm at the laboratory scale. Of particular interest is the region of interaction between plant roots and the water table capillary fringe, which is extremely difficult to study in the lysimeters. It is in this region that redox potential falls rapidly with increasing water content. These column experiments are conducted within plastic columns of 0.5m length maintained in a growth cabinet with full environmental controls. Each column sits in a tray of water contaminated with ^{22}Na, ^{137}Cs and ^{36}Cl. Monitoring of soil moisture profiles is achieved *in situ* using Time-Domain Reflectometry (TDR) probes, which are integral to the structure of the column, and redox potentials are similarly monitored with *in situ* platinum electrodes. The columns are split longitudinally to facilitate sampling of the entire soil column. A typical experimental set up is shown in Plate 9.

Results from the Phase 1 experimental studies are not presented here, as some details are already available in the open literature [142, 143]. Further results will be made available in the same way, when the radiochemical data have been fully quality assured and evaluated. Overall, the results available to date support the concept of tin enhanced efficiency of radionuclide uptake in the vicinity of the water table capillary fringe. Additionally, following absorption by plant roots, internal translocation evidently provides a rapid route by which radionuclides may be transported to the soil surface where, following leakage from plant tissues, they will presumably become available for uptake in subsequent seasons [143].

Plate 9: Column experiment studying radionuclide transport in the laboratory



5.3 Modelling Developments Since 1992

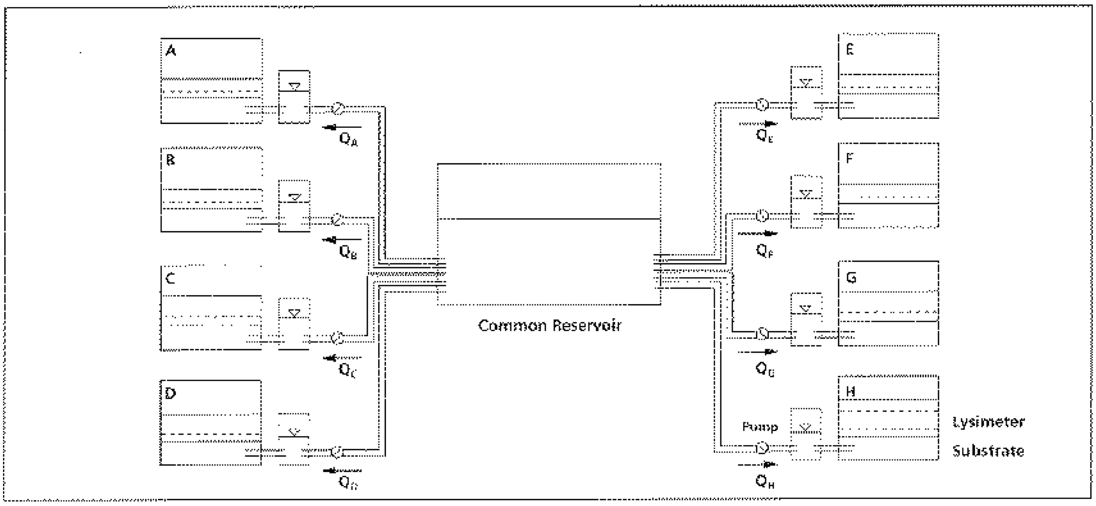
As described in subsection 5.1 a detailed model of coupled soil-plant-water processes (SPW1) was developed in the initial stages of the programme in conjunction with a solute transport model (SLT1). However, the lysimeter experiments themselves are complex, so, to aid data interpretation and quality control a model of the complete lysimeter experimental system has been developed (LYS1), which includes a simplified representation of radionuclide transport and crop uptake.

LYS1 conceptualises the water table control system as a series of connected compartments *(Figure 10)*. Water flow between these compartments is derived from peristaltic pump measurements. Radionuclide transport in the lysimeter soil is conceptualised into an expanding box which is divided into upper and lower zones *(Figure 11)*. The upper boundary of the box moves upwards in response to advective fluxes (due to evapotranspiration) retarded by soil sorption. The region in which infiltrating meteoric water mixes with radioactive water is represented by the upper zone of the box and hence the boundary between the upper and lower zones migrates in response to soil water movement again subject to soil sorption processes. Uptake of radionuclides by the crop is simulated using a linearised root sorption model based on Michaelis-Menten kinetics. The total uptake by the root system is obtained by integrating the specific uptake flux over the entire rooting depth using a root density distribution model calibrated against experimental observations.

The first application of LYS1 was to the first two seasons of data (1990 and 1991) for ^{22}Na. The model was able to simulate successfully the behaviour of ^{22}Na in the various components of the water table control system when calibrated against soil core and harvest crop activity data. The model was also able to reproduce the variability in total crop activity at harvest between lysimeters and to a lesser extent between the two crop seasons. The model was then used to predict ^{22}Na uptake by the 1992 crop and was found to perform satisfactorily *(Figure 12)*.

Subsequently. the LYS1 model was applied to the 1990/1991 data for ^{36}Cl. This work highlighted a significant difference between the amount of ^{36}Cl estimated to be present in the system and the

Figure 10 **Conceptualisation of lysimeter water-level control system. For details of the conceptualisation within a single lysimeter see Figure 11**



amount added. Improved extraction methods have since determined the presence of a fraction of the missing deficit in the SO~1, and tests to determine the reason for the remaining deficit are underway.

In addition, a set of detailed model simulations have been undertaken for both ^{22}Na and ^{36}Cl. SPW1 was used to derive water fluxes and moisture contents, which were then used as input to SLT1, together with other parameter values derived from LYS1 simulations, combined with literature values

Figure 11 **Conceptualisation of radionuclide transport in soil in the lysimeter system model**

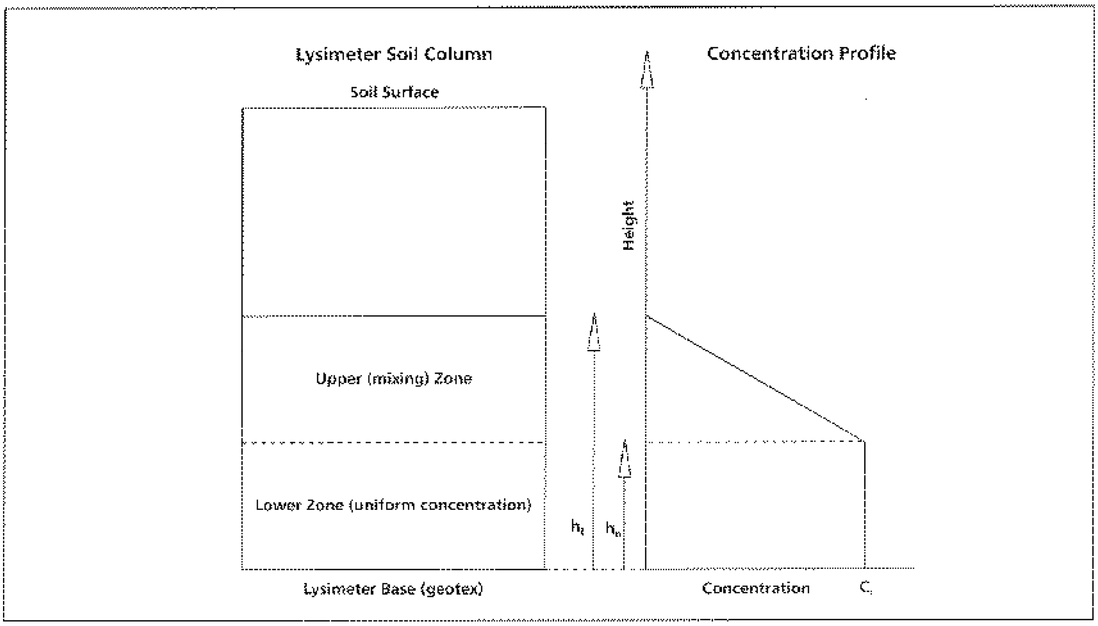
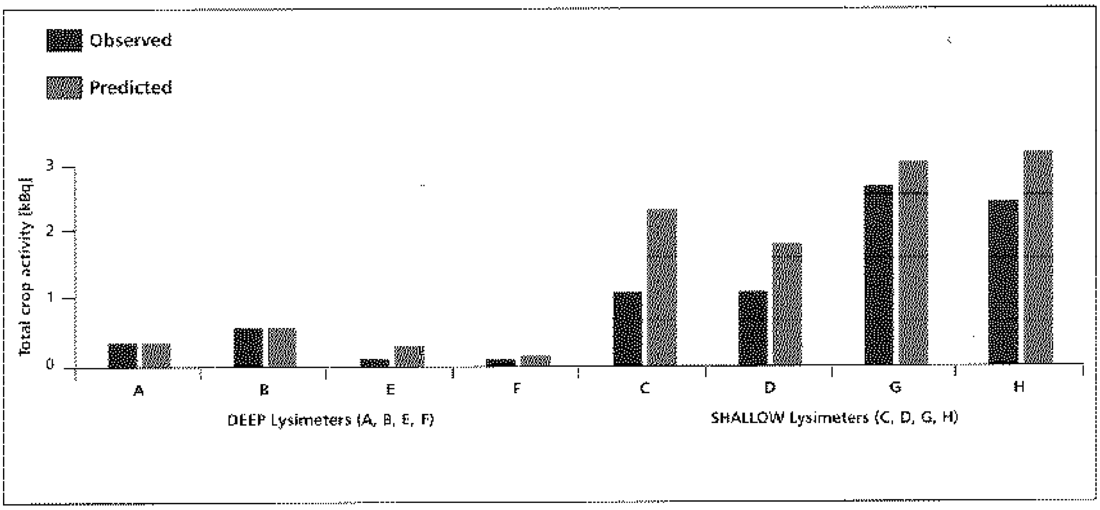


Figure 12 **Observed and predicted uptakes of ²²Na by the 1992 winter wheat crop**



of diffusion and dispersion. The resulting model simulations of the behaviour of ^{22}Na over the 1990 and 1991 seasons for generic deep (0.65m) and shallow (0.35m) lysimeter representations gave broadly encouraging results (*Figure 13*).

A similar study for ^{36}Cl has recently been completed, using hydrological characteristics identical to those adopted for the ^{22}Na calculations. These simulations were able to reproduce the average crop uptakes from the deep and shallow lysimeters for the 1990 and 1991 harvests *(Figure 14)*. The effect of the ^{36}Cl deficit noted above can be observed in the soil profiles, which reproduce the overall form of the soil distribution, but show a

Figure 13 **Observed and predicted distribution of ^{22}Na in deep lysimeter soils for 1990 and 1991**

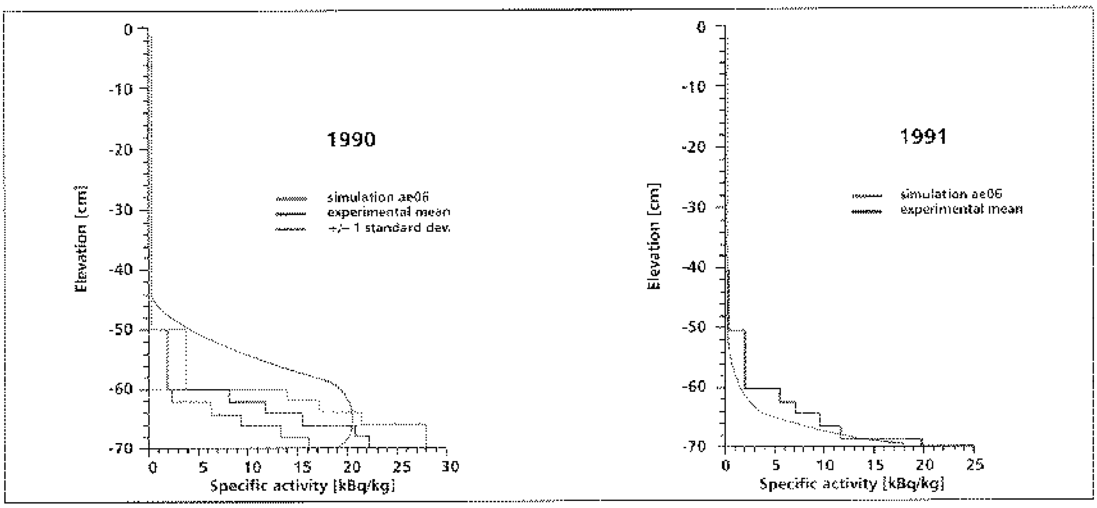


Figure 14 Observed and predicted uptakes of ^{36}Cl by the 1990 and 1991 winter wheat crops

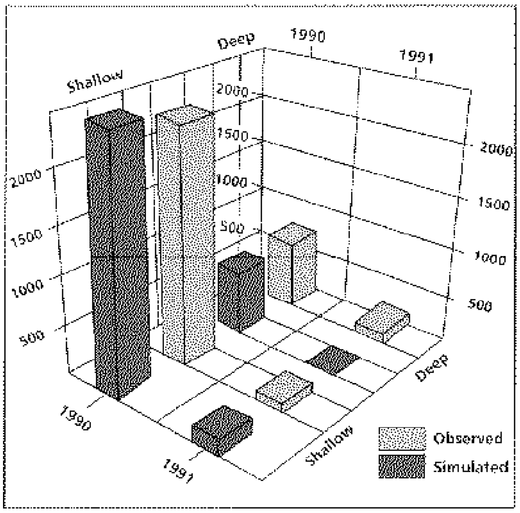
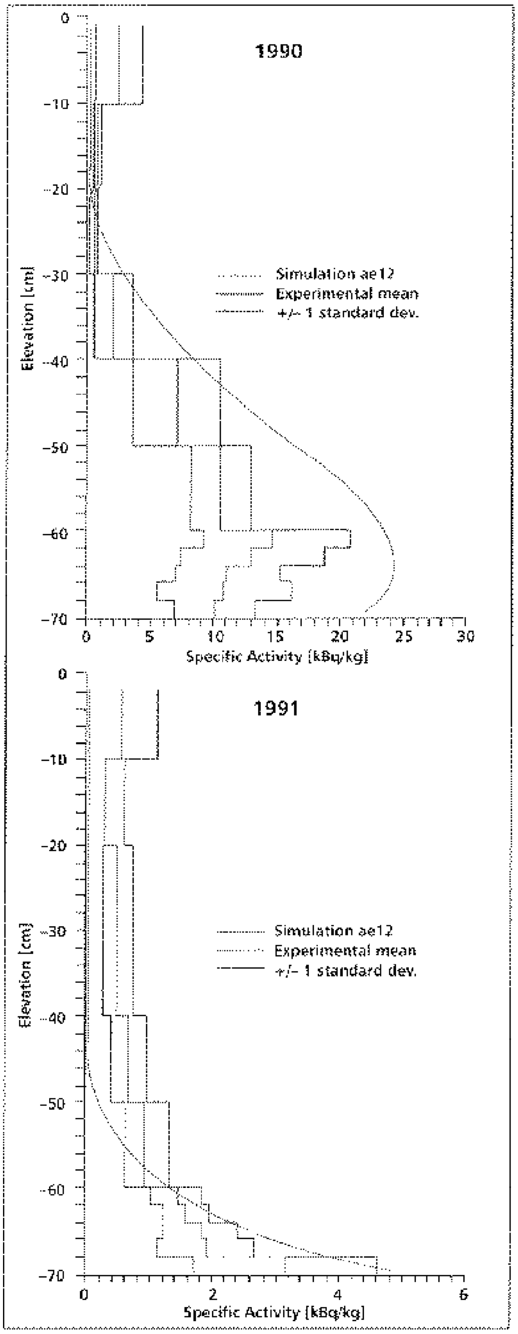


Figure 15 Observed and predicted distribution of ^{36}Cl in deep lysimeter soils for 1990 and 1991

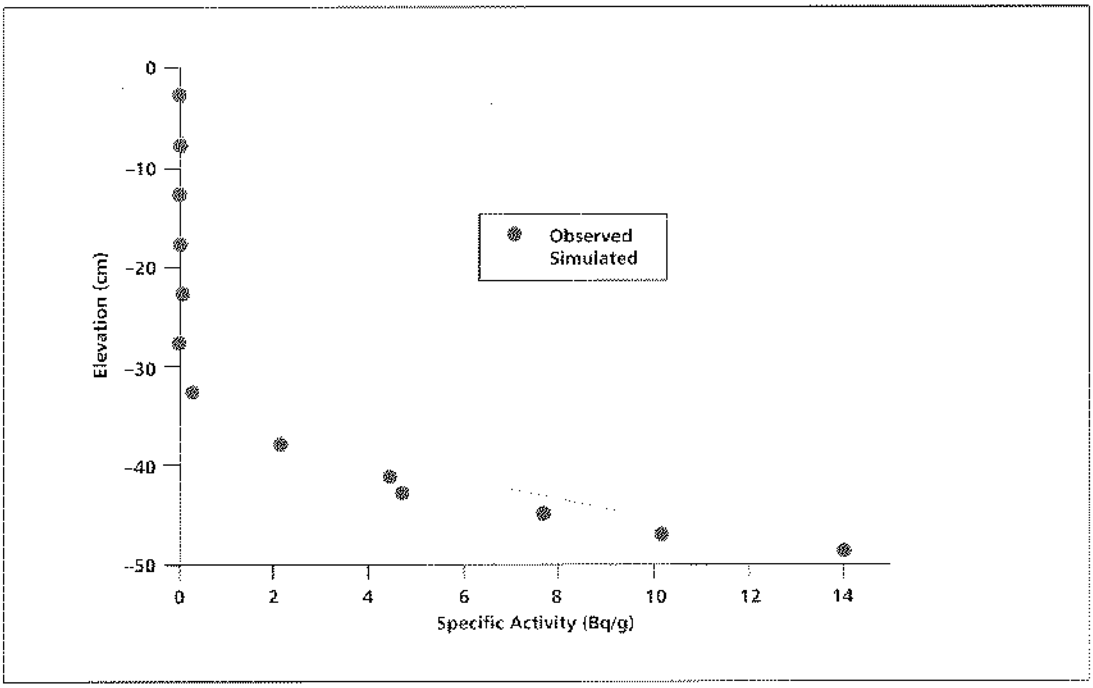


consistent over-estimation *(Figure 15)*.

Notwithstanding these encouraging results, there are some differences between the SLT1 simulation results and the experimental data which need to be addressed. Specifically, lysimeter core samples for 1990, 1991 and 1992 show concentrations of residual activity remaining in the upper portion of the soil profile which are not reproduced by the model simulations, and this can lead to some degree of underestimation of crop uptake. It is considered that this arises partly because SLT1 is a single-porosity model. For this reason a new version of the model (SLT2) has been produced, which incorporates a dual-porosity approach. In addition, consideration is being given to introducing various biological transfer components into this new dual-porosity model. These include root storage release due to root rotting, litter fall and leaf wash-off.

Finally, it is noted that the detailed models have also been used to simulate the movement and uptake of ^{22}Na in column experiments. In these

Figure 16 Observed and predicted distribution of ^{22}Na in a column experiment conducted in the laboratory



studies, excellent reproduction of the activity profile observed in the column has been achieved *(Figure 16)*. It is emphasised that this simulation uses the hydrological and solute transport parameters derived for the lysimeter simulations, the only exception being the root sorption coefficient, which was increased. The need to increase the sorption coefficient may be attributed to differences between spatially constrained and unconstrained root systems. Overall, the consistency of data from the lysimeters with data from the column experiments provides an encouragement to the more extensive use of column experiments in the future.

5.4 Status of the Research and its Relationship to Assessments

The Phase I lysimeters have provided a unique opportunity to study the processes of radionuclide distribution and transport in soils contaminated from below. Encouragingly, models formulated on relatively conventional lines (single or dual porosity, with root uptake governed by Michaelis-Menten kinetics) have been sufficient to represent most aspects of the experimental data. Overall, the major new findings to emerge have been the high efficiencies of plant uptake that can occur in dry conditions, the importance of climatic variability and the significant translocation of strongly sorbed chemical species.

Processes of transfer are now being explored in column experiments complementary to the lysimeter studies. In this context, it is encouraging that the same models, and generally the same parameter values, can be used to interpret both the lysimeter and column experiments.

Some of the limitations of the original lysimeter experiments, *eg* use of a fixed water table, are being overcome by the variant studies undertaken during the fifth full season of the experiment. However; assessment studies undertaken since the programme was initiated in 1988 have demonstrated that whereas arable food chain pathways are of interest for a variety of radionuclides, the transfer of ^{36}Cl via the pasture-cow-man pathway is of overall greater importance [1]. Thus, although ^{36}Cl was included in the Phase 1 study, the choice of winter wheat as a crop was not ideal.

Also, the Phase 1 experiment was undertaken using the rather sandy, local soil available at Silwood Park. Although this soil type is directly relevant to the Brown Earths and Sands found in the Sellafield area [144], it was recognised that there is a need to explore a variety of soil types relevant to post-closure radiological performance assessments [1].

For these various reasons, a Phase 2 lysimeter experiment has been planned and is currently being set up. This has the objectives of:

- Extending the experimental database to include a perennial, pasture species, since plant uptake processes are known to be strongly dependent on plant type, and, in particular on the dynamic interactions between root development and distribution, and hydrological conditions;
- Comparing soil transfers and plant uptake in two contrasting soil types, one of which should he from the Sellafield area;
- Providing models and data relating to ^{36}Cl distribution and transport in soils and uptake by pasture plants, since ^{36}Cl is identified as a key radionuclide in post-closure radiological performance assessments, with the dominant pathway of exposure being the pasture-cow-man foodchain.

As in Phase 1, eight lysimeters are being used, but, in this case, all with a water table of 0.65m depth. Four of the lysimeters are filled with the sandy loam Silwood Park soil, whereas the other four are filled with a clayey/silty soil from Longlands Farm near Sellafield, which is where much of the Nirex deep geological Site Characterisation programme is centred. In all eight lysimeters, perennial rye grass will be grown. Thus, comparisons will be possible on the effects of crop type (rye grass and wheat on Silwood soil) and soil type (rye grass on Silwood and Longlands Farm soils).

By July 1994, the new set of lysimeters had been fully refurbished and were being filled with soil. Three months are being allowed for soil settlement, and control systems are to be transferred following the final Phase 1 harvest. The crop will be established over the autumn/winter of 1994. Radionuclide dosing, with ^{36}Cl and ^{137}Cs (as an extensively studied, control radionuclide), will take place in March/April 1995, to coincide with the onset of net upward flux conditions. Three crop seasons, 1995, 1996 and 1997 are planned, with decommissioning and destructive analysis over the period October 1997 - March 1998.

It is intended that these studies will provide additional data on the dynamics of ^{36}Cl in soils and uptake by plants. As with the data and model interpretations available to date, these will be used in specifying input data for the catchment-scale simulations used in direct support of post-closure performance assessments (*see subsection 4.4 and* [1]). In addition, the data and models are providing an input to the international BIOMOVS II programme [1].

6 Relationships to other Research Programmes

As demonstrated in Sections 2 to 5, the overall scope of the biosphere sector of the NSARP includes studies in climatology, landform evolution and near-surface hydrology, designed to provide a context for modelling the distribution and transport of radionuclides in the future environments that may occur at Sellafield. Many of the issues being addressed are of interest in a wider context than radioactive waste disposal, so it is important that the various projects in the biosphere sector establish appropriate links to the wider research community.

In the context of climate and climate change, the need for establishing these wider links was recognised at an early stage. Thus, on completion of the initial review study 151, an international workshop was organised to compare the approach being adopted in the Nirex programme with other approaches being adopted in the UK and in other countries, notably France, Belgium and the USA 11451. Subsequently, close links were maintained with Belgian and French groups pursuing work of particular interest to Nirex, which has now led to collaborative work on climatic modelling and on the use of indicators from terrestrial sediment cores to reconstruct palaeotemperature and precipitation histories for a site on the Atlantic Margin of northwest Europe (*see subsections 2.4.1 and 2.4.2)*. In parallel, the Climatic Research Unit, University of East Anglia (CRU), who undertake the majority of the Nirex climate studies, have maintained close links with a variety of research institutes worldwide, notably the National Geophysical Data Center, Boulder, Colorado, which maintains an archive of relevant palaeoindicator data. In addition, access to the most recent research into, and results from, transient GCMs is provided through the CRU/ Hadley Link Project funded by the UK Department of the Environment [57].

Work on landform evolution tends to be more regional, or site, specific than work on climate change. For these reasons, links with overseas research are not as well-developed in this area as they are in climatic studies. Nevertheless, reference is made to overseas work where it provides insights into processes of relevance in Cumbria. Thus, for example, the study on Glacial Britain [74] notes that White [146, 147] has set out an account of the glaciation of North America that closely parallels that developed for the British Isles, draws attention to related Norwegian work on Quaternary erosion [148, 149], and identifies supportive comments arising from studies of the sedimentary record of the Antarctic continental shelf [150] . However, overall, it is considered more important that the work on landform evolution should be reviewed by British experts with field experience of the areas under discussion (see e.g. the acknowledgements in [74]), and should take account of British field studies by overseas experts who often bring a different perspective to our landscape and its origins (*see, eg* [151 - 153]).

Research on near-surface hydrology necessarily relates to a wide, international, on-going programme. As mentioned in subsection 4.1, the SHE model on which SHETRAN-UK is based, was developed jointly by the Danish Hydraulic Institute, the British Institute of Hydrology and SOGREAH (France). In the UK, the Water Resource Systems Research Unit (WRSRU), which undertakes SHETRAN-UK developments, also has general responsibilities for the development, maintenance and application of SHE. This work is done in close administrative collaboration with their Danish and French co-developers.

As a water resource tool, SHE is in demand worldwide with model tests and applications relating to catchments in the UK, New Zealand, Switzerland, Thailand, the United States of America, Germany, Spain, Portugal, France, Denmark, Italy and India. The close relationships established with research institutions in the partner countries and elsewhere have been a convenience in obtaining data for use in validation studies (from Rimbaud, France and Upper Sheep Creek, USA) and in simulations of hypothetical catchments designed to be characteristic of the Sellafield area in future boreal conditions (from Kotioja, Finland) [1].

The general interest in large-scale, nearsurface, hydrological modelling, and the high reputation that the WSRU has in this area, are reflected in the broad base of funding which exists for development of the macromodel, with contributions from the Natural Environment Research Council and the European Commission. Furthermore, these developments are taking place within a unit which collaborates with a wide variety of organisations on water resource and contaminant transport issues. Similarly, the work on intact cores and field plots is located within the Centre for Research on Environmental Systems (RES) at University of Lancaster, which has an international reputation in this area.

The lysimeter system set up at Silwood Park was recognised from the outset as a unique facility worldwide. Throughout Phase 1 of the experiments, discussions of the work have taken place with interested colleagues in China, France, the United States of America and Canada. In addition, Principal Investigators from the project are members of the International Union of Radioecologists (IUR) and results from the work are made available to that group. In the UK, annual accounts of the various experimental and modelling studies are given to the Natural Environment Research Council Co-ordinating Group on Environmental Radioactivity (COGER). More recently, results from the lysimeter experiments have been made available to the international biosphere modelling programme BIOMOCS II for use in model validation studies [1].

Overall, the carrying out of NSARP biosphere research, largely in specialist units within a university context has done much to encourage both formal and informal links with related research activities in the UK and overseas. These links are further encouraged by a policy of publishing results from the research not only in freely available research reports, but also in books, conference proceedings and refereed journal articles (see bibliography).

7 Summary

The overall scope of the biosphere sector of the NSARP has not changed markedly since 1992, with attention remaining concentrated on climatology, landform evolution, near-surface hydrology and contaminant transport, and radionuclide migration in the near-surface soil zone, including uptake by plants. However, within each of these areas, progress has been rapid, resulting in a variety of new issues being raised and addressed, and new activities being undertaken.

In climatology, the continued rapid pace of developments worldwide makes a component of literature review essential to the programme. However, the published literature has limitations as a basis for post-closure radiological performance assessments. In particular, the experimental data collected and model simulations undertaken are unrelated to questions specific to the Sellafield area. Indeed, many of the available data and model results do not even relate specifically to the Atlantic Margin of northwest Europe. Additionally, limitations of space often constrain published articles to providing summaries of experimental data or model results, where the comprehensive datasets acquired would be more useful for analysis and interpretation in a local or regional context. For these reasons, and because attention is now directed firmly at Sellafield as the single site being subject to detailed characterisation, it has been determined that a more active role should he taken in the acquisition and interpretation of relevant palaeoindicator data, and in the simulation of potential future climatic evolution at Sellafield. This has led to the acquisition of detailed archives of palaeoindicator data from the National Geophysical Data Center, Boulder, Colorado and from other sources, the initiation of coring at Dingé, and the setting up of a programme of model simulation studies in collaboration with the University of Louvain-la-Neuve (*subsection 2.4)*. The central component of this programme is to perform simulations covering the next 100,000 years to provide estimates of global ice volume, and monthly and annual temperatures in different latitude bands *(subsection 2.4.1)*. These results will then be used via a downscaling approach that is currently under development, to provide values of temperature and precipitation, on a seasonal and/or monthly basis, appropriate to the Sellafield area.

In the first instance, these 100,000 year simulations will neglect the effects of anthropogenically induced increases in greenhouse-gas concentrations, which will be taken to vary with time only as a consequence of the antecedent climatic conditions. However, in parallel, studies will be undertaken to determine the degree to which the climate system would be perturbed over the next 500 years if various of the IPCC scenarios were assumed to occur. This will give a basis for discussion as to how those scenarios should l}e extended to provide a forcing function that can he applied in long-term simulations.

Overall, although the unresolved issues relating to climate identified in 1992 *(see subsection 1.1)* have not been fully resolved, enough progress has been made for it to he appropriate to move from describing possible future climatic conditions to attempting to model potential patterns of future climatic change. The IPCC scenarios provide an internationally recognised basis for assessment, though they themselves are subject to change and do not extend as far into the future as required. In addition, a model is now available which includes a reasonable degree of physical realism, and can be forced by both insolation variations and changes in greenhouse-gas concentrations. Nevertheless, it is emphasised that not all processes of potential significance are incorporated in that model, and that substantial scientific issues remain outstanding in respect of the characteristics of the global carbon cycle and the response of the climate system to various forcing and feedback factors, such as vulcanism and sulphate aerosols *(subsection 2.3)*.

In respect to landform evolution, the view expressed in 1992 was that proposed patterns of landform evolution prior to, and, more particularly, subsequent to, any future glaciation must be considered highly speculative. However it was also indicated that more quantitative studies would be instituted when this became appropriate.

Subsequently, the review of Glacial Britain that has been undertaken has provided an overall conceptual model of how glacial erosion and deposition operates, and has generated quantitative estimates of the overall amount of glacial erosion per glacial/interglacial cycle. This work has emphasised the major (or even dominant) role of glacial episodes in the denudation of Northern Britain over the period of the Quaternary *(subsection 3.2)*. Projected into the future, this interpretation of the role of glacial processes leads to an anticipated average lowering of the Cumbrian land surface by about 200m over the next one million years *(subsection 3.2.2)*. However; the highly incised nature of the current land surface, as well as the relief contrast between the uplands and the coastland lowlands, suggests that significant spatial variations in the degree of surface lowering will exist. A first attempt to quantify these spatial variations has been made, based on analyses of data included in the digital relief map *(subsection 3.3)*. This initial study indicates that the relief contrast between the Lake District and the surrounding lowlands has been increased by Quaternary glacial erosion. This reached an average depth of only 120m on the Lower Palacozoic rocks. On the surrounding rocks, erosion was of the order of 100m on the higher ground, but reached 650m in the deeper glacially eroded basins. The degree to which this process of differential erosion will continue under potential patterns of future climate change for the region remains to be explored.

These studies have emphasised the importance of glacial episodes as determinants of both general and localised erosion. However, such episodes are also of significance through their influences on the hydrogeology of the region and in consequence of the isostatic depression of the Earth's crust due to ice loading. For these various reasons, it is important to have an adequate understanding of the dynamics of the growth and decay of British ice sheets. A review of mathematical approaches to the modelling of ice sheet dynamics had revealed, by the time of the last review, that existing models may be inadequate for representing evolving conditions in the Sellafield area *(see subsection 3.4)*. The model comparison exercise currently being undertaken should shed some light on this matter.

The ice sheet model intrinsically generates temperature and pressure fields at its base which can be used as inputs to groundwater modelling. These temperature and pressure fields are conditioned by the basal sliding law assumed, and the effects of adopting alternative basal sliding laws may readily be addressed in sensitivity studies, as required. Furthermore, the current model comparison exercise is for the case of an ice-sheet with a non-deformable bed and extension to the case of isostatic deformation, including both depression beneath the ice sheet and possible forebulge effects, is a logical next step. In this context, it is encouraging to be able to report that crustal depression and recovery with ice sheet loading and unloading has been studied in some detail for the British Isles, with account having also been taken of the loading of the sea floor by water *(subsection 3.4)*. However, though there is generally good agreement between observations and theory, there remains room for improvement, with the northwest coast of England, the Isle of Man and the Solway Firth identified specifically as an important area for further investigation.

Isostatic depression from ice loading, subsequent recovery, and other neotectonic movements, may occur aseismically, or through movement on pre-existing faults. The digital relief map which can be used to indicate areas of uplift bounded by specific known faults is a useful development, although currently no model is available to estimate the likely degree of such movement under various patterns of loading and unloading.

Overall, the research projects in climatology and land-form development are moving forward rapidly into a quantitative phase in which:

- Long-term climate modelling is used to provide potential patterns of future climate at global and coarse regional scales;
- Downscaling of the results of the long-term climate modelling is used to provide potential patterns of future climate at the regional and local scales;
- These patterns of future climate are used to estimate variations in global sea level, as well as spatial and temporal patterns of erosion;
- In addition, the patterns of future climate are used to determine the likely evolution of ice sheets in the British Isles, in general, and in Cumbria, in particular;
- Ice sheet loading and sea level variations are used to compute isostatic responses and hence to determine regional sea level;
- Climate, sea level, ice sheet and topographic variables are used, in conjunction to generate time-dependent boundary conditions for groundwater modelling, and to determine the broad characteristics of the biospheres into which radionuclides may emerge.

At the moment, developments in each of these areas are at an early stage, but, over the next few years, the links between these various aspects of the future evolution of the environment at Sellafield are expected to be considerably strengthened.

In this context, it is relevant to note that research in these various areas will rely heavily on data now beginning to emerge from the Quaternary component of the Site Characterisation programme. As pointed out in subsection 3.5, the existing drift deposits onshore and offshore at Sellafield provide extensive evidence on the history of the area subsequent to the Last Glacial Maximum and this evidence is directly relevant to assessing how the environment may develop subsequent to future glacial episodes. Furthermore, it is possible that these sediments may provide clues to any post-glacial fault movements in the area, either through fault displacements which propagate through the sediments and/or through sediment convolutions that can be interpreted as evidence of seismically induced liquifaction.

Overall, the work on climatology and land-form evolution is designed to provide a context for modelling both the deep and near-surface hydrological regimes. Deep hydrology and hydrogeology is an aspect of the geosphere sector of the NSARP [2], but near-surface hydrology and radionuclide transport are included in the biosphere sector.

The principal tool used in modelling near-surface hydrology and radionuclide transport is SHETRAN-UK. The current production version of this program (Version 3.4) was available in 1992, and much of the subsequent work has related to validation of the flow and transport components of the program, and to its application in assessment-oriented studies of hypothetical boreal and temperate catchments.

In respect of validation, the period since 1992 has seen the first full application of the blind validation methodology to water flow characteristics of the Rimbaud catchment *(subsection 4.2)*. Although the preset criteria for successful validation were achieved in only one out of the four tests, this was the first time a test of this rigour had ever been applied to a hydrological model, and the study has therefore given considerable confidence in the predictive capability of SHETRAN-UK. Specifically, the capability of SHETRAN-UK to simulate the interactions between surface and subsurface runoff for storms of greatly differing magnitude was demonstrated, while the aspects of the model that led to over-predictions of storm peaks and the undue sharpness of the subsequent recessions were readily identified.

The period since 1992 has also seen the development of a capability to validate SHETRAN-UK against contaminant transport experiments at the field-plot scale. The first series of such experiments involved the use of conservative tracers at the Hazelrigg Field Station, University of Lancaster These have now been completed, as have initial simulations of them using SHETRANUK. However, the studies at Hazelrigg were, in many respects, only a test of the full field-plot methodology, which is now being implemented at Calder Hollow, Sellafield. The experiments at Calder Hollow, which are now under way, include studies with conservative, weakly sorbing and strongly sorbing tracers, complemented by blind validation studies.

Although the current version of SHETRAN-UK provides an extremely useful tool for exploring water flow and radionuclide migration in a wide range of different catchment types, there are three areas in which developments of, or extensions to, the system have been identified as desirable *(subsection 4.3)*. The first of these, a new variably saturated subsurface component of the model to represent more adequately areas of complex lithology, has already been designed and is currently being implemented in a development version of the code, which is scheduled to become the production version in April 1995 *(subsection 4.3.1)*. The need for this new component was recognised before the results of the Rimbaud validation study became available, and was confirmed by those results.

The second development is incorporation of a cold-region component into the model to represent frozen-ground effects. Because this component requires access to some facilities developed for the variably saturated subsurface component, it has been carried forward only to the review stage so far.

Finally, there is a requirement to extend the timescale of modelling from decades to centuries. This is being achieved through the development of a general purpose macromodel capable of predicting flow and transport for larger areas and longer time spans than can SHETRAN-UK. Work on the water-flow component of this macromodel is well advanced, and, while work on the contaminant transport component is at a relatively early stage, a combination of particle tracking and finite-difference techniques has been demonstrated successfully *(subsection 4.3.3)*.

SHETRAN-UK has also been used extensively in assessment-related studies of hypothetical boreal and temperate catchments, providing useful insights into the modes of use of the model, and techniques of post-processing the results, that are particularly useful for assessment purposes. The availability of the model also provides a context for near-surface geological and hydrological data arising from the Site Characterisation programme. Thus, it is foreseen that the temperate catchment description will be refined, using these data, until it can properly be characterised as a near-surface hydrological model of the site at the present day. Variants of this model will then be used to represent potential future temperate catchments in the vicinity of the site *(subsection 4.4)*.

A key area of uncertainty in catchment-scale modelling is the transport of radionuclides in the soil zone when contamination is from below. Over the last seven years, this issue has been addressed through a programme of experimental studies on radionuclide transport in large soil-filled, vegetated lysimeters, complemented by detailed modelling studies. The objectives of this programme are to determine and investigate the key processes governing radionuclide distribution and transport in soils, and to characterise these processes for radionuclides of particular importance In assessments.

By 1993, the projected four full seasons of data had been obtained from the Phase I lysimeters running in the original mode of operation *(subsection 5.2)*. Subsequently, these lysimeters have been used, in the fifth and final year of the experiment, to explore some of the questions raised by the project that it had not been possible to investigate in the original mode of operation. In addition, in order to study radionuclide transport processes in more detail than is possible in the full-scale lysimeter experiment, a series of column studies have attempted to reproduce the lysimeter system in microcosm at the laboratory scale.

Overall, the results of the Phase 1 lysimeter experiments and supplementary column studies support the concept of an enhanced efficiency of radionuclide uptake in the vicinity of the water table capillary fringe. Additionally, following absorption by plant roots, internal translocation evidently provides a rapid route by which radionuclides may be transported to the soil surface.

Models available to interpret the various experiments included detailed 1-D soil-plant-water and solute-transport models, the second of which has recently been modified from a single to a dual porosity representation in order to account for the available experimental data *(subsection 5.3)*. In addition, to aid data interpretation and quality control, a model of the complete lysimeter experimental system has been developed. This has proved invaluable, especially as large amounts of radiochemical data have now been accumulated. In particular the model has been used, successfully, to reproduce the variability in total crop activity at harvest between lysimeters and, to a lesser extent, between crop seasons, for ^{22}Na and ^{36}Cl. Soil transport and plant uptake of these two radionuclides have also been studied using the 1-D detailed models.

Although some of the limitations of the original lysimeter experiments are being overcome by the variant studies undertaken during the fifth full season and by the complementary column studies, there are some issues which can only be addressed in a different system configuration. Specifically, assessment studies undertaken since the programme was initiated in 1988 have demonstrated the need to study transfers of ^{36}Cl in pastures characteristic of the Sellafield area. Thus, a Phase 2 lysimeter experiment has been planned and is currently being set up *(subsection 5.4)*. This has the objective of extending the experimental database to include a perennial pasture species; comparing soil transfers and plant uptake in two contrasting soil types, including one from the Sellafield area; and providing models and data relating to ^{36}Cl distribution and transport in soils, and uptake by pasture plants.

In conclusion, all the outstanding issues identified in the biosphere sector of the NSARP in 1992 have been addressed in the studies undertaken subsequently. Although it cannot be stated that these issues have been fully resolved, the outstanding questions are now much more sharply focused. This parallels a general move in the biosphere sector away from review and descriptive studies, and towards quantitative modelling. This trend is likely to continue over the next few years, allowing traceable quantitative arguments to be developed relating climate change to landform evolution, which together will provide a time-dependent context for modelling radionuclide transport through a changing environment. This modelling will include transient groundwater flow and transport calculations, with boundary conditions provided from the various biosphere studies (including ice sheet simulations), near-surface catchment-scale studies, using SHETRANUK for detailed snapshots of system behaviour and the macromodel for longer-term simulations, and a variety of assessment-related studies using the time-dependent model being developed as part of the DSAT programme [11.

Also, the period since 1992 has seen an increasing emphasis on site-specific studies. Thus, both the climate and landform evolution projects have concentrated on aspects specific to Cumbria, hypothetical catchment studies are for catchments considered to be characteristic of the Sellafield area, field plot experiments have moved from Lancaster to Sellafield, and lysimeter experiments are now using soils taken from the Nirex site at Longlands Farm. Another aspect of this trend has been an increasing involvement with Site Characterisation activities, notably studies on the drift deposits *(subsection 3.5)* and the programme of near-surface hydrological characterisation *(subsection 4.4)*. This trend towards site-specific work is also likely to continue over the next few years, so that the modelling studies outlined above will be increasingly driven by site-specific, and not generic, data.

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