



**British  
Geological Survey**

NATURAL ENVIRONMENT RESEARCH COUNCIL

# DAEM Model Inventory

Data and Applications for Environmental Modelling Programme  
Open Report OR/10/010



# DAEM Model Inventory

A Barkwith

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## Keywords

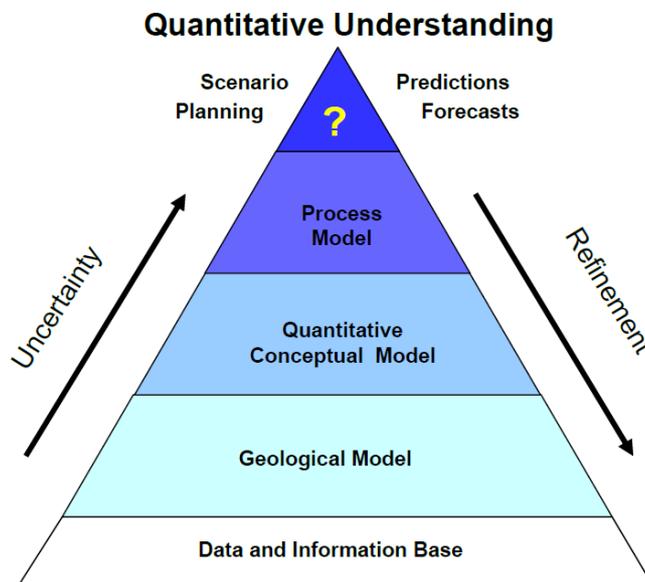
Earth Systems Model, NERC, Integrated modelling, Inventory.

## Bibliographical reference

A BARKWITH. 2010. DAEM Model Inventory. *British Geological Survey Open Report*, OR/10/010. 97pp.

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# 1 Introduction

As part of the BGS strategy (BGS, 2009) the need to develop an Environmental Modelling Platform (EMP) has been identified. The Data and Applications for Environmental Modelling (DAEM) project has sought to scope out the requirements for an EMP. The DAEM project has four deliverables: a scoping study, an outline project plan for the next five years, a model inventory of model codes currently used within NERC, and community building. The scoping study together with the plan for the next five years has been published as a separate document (Giles et al., 2010).

This report, an inventory of current Earth science models (and code) used by NERC centres, was created to form part of the appendices for the scoping study (Giles et al., 2010), but has since been commissioned as a separate report. The description for each model has come from the NERC institute indicated in the report. Where a description has not been given, a web search was used to compile the model information. Earth system modelling is undertaken at the majority of NERC centres, however where no information was given, found, or if no models are used, that centre has not been included in this report.

Each entry contains a brief description of the model background, capabilities, and references to further information. The contact and use given for each model is specific to that NERC centre or department and therefore there are occasions where the same model is referenced more than once. The NERC contact cited has some degree of experience in using the model and in most cases should be able to answer related questions or direct queries to a suitable person if the required information can not be found via the link provided. The code language and runtime platform are included to aid with determine the ease of model linkages.

As many relevant staff in the NERC centre/surveys were approached and consulted as possible. Whilst every effort has been undertaken to ensure the accuracy and completeness of this report, it is not necessarily comprehensive and the DAEM project team apologises in advance for any omissions.

## 2 Overview

The following table provides an overview of the model codes identified as part of the review and the part of NERC that uses and/or developed them. Further details can be found in Section 3 onwards.

Model Name	BAS	BGS	CEH	POL	Collaborative Centres
AT123D		X			
BASFOR			X		
BASGRA			X		
BASISM	X				
BERJFUN	X				
BGGM		X			
BGSPT		X			
BIOMOC		X			
BIOSCREEN		X			
BLASIOUS					X
CAF2007			X		
CASCADE-N			X		
CHAIN2D		X			
CHIME					X
CICE					X
CLASSIC			X		
COLUMN2		X			
CXTFIT		X			
DEPOMOD					X
DRIED-UP			X		
DyDOC			X		
ERSEM					X
FATMIC		X			
FEFLOW		X			
FLUVSIM		X			
FOAM				X	
FORTE					X
FRAME			X		
FTRANS		X			
GCOMS					X

Model Name	BAS	BGS	CEH	POL	Collaborative Centres
GLOMAP					X
GOCAD		X			
GOTM-ERSEM					X
GS13D		X			
GW25D		X			
GWAVA			X		
HADAM3	X				
HADCM3	X				
HTS3D		X			
HWM(93 and 07)	X				
HyCOM					X
HYDRAQL		X			
HYDROTHERM		X			
HYDRUS-ID		X			
ICOM				X	X
IGCM					X
IGCM3	X				
IGRF		X			
IHDM			X		
JULES			X		X
Landscape Evaporation			X		
Layered-R- $\Theta$ Model		X			
LEM					X
LF2000-WQX			X		
LIM					X
MARKAL					X
MDM-E3					X
MECOSIM		X			
MEDUSA					X
MICOM					X
MINEQL		X			
MITGCM				X	X
MODFLOW		X			
MODPATH		X			
MOM				X	

Model Name	BAS	BGS	CEH	POL	Collaborative Centres
MRCS/Atlantic Margin					X
MT3D		X			
MT3DMS		X			
NAPL (2D/3D)		X			
NEMO				X	
NEMO_ERSEM					X
OCCAM					X
OCCAM 2D				X	
OpenMI		X	X		
OSMOD		X			
p-TOMCAT	X				
PEARLS			X		
PHAST		X			
PHREEQC		X			
POLCOMS				X	
POLF		X			
PROTECH			X		
PSISM	X				
QUESTOR			X		
QUODDY				X	
R GWL Simulator		X			
Radial Flow Model		X			
ReFH			X		
RIVPACS			X		
ROMS				X	
RT3D		X			
RWEQ		X			
SCAMP			X		
SEAWAT-2000		X			
SEEP2D		X			
SOLMAG AND PDFLAP		X			
STAFAN		X			
SUPCRT		X			
SUTRA_MS		X			
SWIFT		X			

Model Name	BAS	BGS	CEH	POL	Collaborative Centres
SWIMIC		X			
SWMS (2D/3D)		X			
TELEMAC				X	
THERMIC		X			
TOMCAT (SLIMCAT)		X			
TOUGH2					X
TRANS1D		X			
TRIANGLE		X			
TRIPM		X			
UK Storm Surge		X			
UKCA				X	
UM					X
Uncertainty Estimation	X				X
UNSAT-H		X			
UTCHEM		X			
UWB 1DV		X			
WATEQ4				X	
WCH		X			
WHAM					X
WMN		X	X		
WRF		X			
ZETUP		X			
ZOODRM		X			
ZOOM_Viewer		X			
ZOOMQ3D		X			
ZOOPT		X			

## 3 NERC RESEARCH CENTRES

NERC's wholly owned research centres provide leadership to the UK environmental science community and play significant and influential roles in international science collaborations.

### 3.1 BRITISH ANTARCTIC SURVEY

The British Antarctic Survey (BAS), based in Cambridge, United Kingdom, has for over 60 years, undertaken the majority of Britain's scientific research on and around the Antarctic continent. It has a long and distinguished history of carrying out research and surveys in the Antarctic and surrounding regions, undertaking most of the British research on the frozen continent. The close linking of its science programmes with essential logistics support makes it effective in carrying out the complicated and sophisticated scientific field programmes that are necessary today.

#### 3.1.1 Climate

##### 3.1.1.1 HWM (93 AND 07)

HWM93 and HWM07 are empirical models of horizontal winds in the troposphere, stratosphere, mesosphere, and thermosphere. HWM07 is provisional and succeeds HWM93 (which was successively based on HWM87 and HWM90). In addition to the radar, rocket and CIRA data used in HWM93, HWM07 is based on extensive new ground-based and space-based wind measurements, including height profiles from NASA-UARS/WINDII, NASA-UARS/HRDI, measurements from ground-based optical and radar instruments obtained from the NSF-CEDAR database, and lower atmospheric NCEP data. The models are maintained through National Space Science Data Centre (NSSDC) in the USA. At BAS the models are used by Rob Hibbins, Martin Jarvis and Tracy Moffat-Griffin.

<b>Model</b>	HWM (93 and 07)
<b>Contact</b>	Martin Jarvis - mjja@bas.ac.uk
<b>Link</b>	<a href="http://nssdcftp.gsfc.nasa.gov/models/atmospheric/hwm07/readme.txt">http://nssdcftp.gsfc.nasa.gov/models/atmospheric/hwm07/readme.txt</a>
<b>Literature</b>	<p>Hedin A. E., Spencer N. W., and Killeen T. L., 1988: Empirical Global Model of Upper Thermosphere Winds Based on Atmosphere and Dynamics Explorer Satellite Data. <i>J. Geophys. Res.</i>, <b>93</b>, 9959-9978.</p> <p>Hedin A. E., <i>et al.</i>, 1996: Empirical Model of the upper atmosphere. <i>J. Atmos. Terr. Phys.</i>, <b>58</b>, 1421-1447.</p> <p>Drob D. P., <i>et al.</i>, 2008: An Empirical Model of the Earth's Horizontal Wind Fields: HWM07. <i>J. Geophys Res.</i>, <b>113</b>, doi:10.1029/2008JA013668.</p>
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows, Linux
<b>Latest Update</b>	2008

### 3.1.1.2 IGCM3

The Intermediate Global Circulation Model 3 (IGCM3) simulates the global dynamics of the Earth's troposphere and stratosphere. It is based on the spectral primitive equation model by Hoskins and Simmons (1975), and includes simple parameterizations of radiation, convection, surface-atmosphere interaction processes (land and ocean), and effects of gravity wave breaking. The model is the most advanced in a range of simplified atmospheric circulation models that have been developed at Reading University, making it of intermediate complexity, in between simple dynamical models and full global circulation models. At BAS the model is used by Ingrid Cnossen, in collaboration with Hua Lu (BAS), Lesley Gray (Reading University) and Chris Bell (Reading University).

<b>Model</b>	IGCM3
<b>Contact</b>	Ingrid Cnossen - inos@bas.ac.uk
<b>Link</b>	<a href="http://www.met.reading.ac.uk/~mike/dyn_models/igcm/">http://www.met.reading.ac.uk/~mike/dyn_models/igcm/</a> <a href="http://www.meteo.mcgill.ca/bourqui-wiki/doku.php">http://www.meteo.mcgill.ca/bourqui-wiki/doku.php</a>
<b>Literature</b>	Hoskins B. J., Simmons A. J. 1975: A multi-layer spectral model and the semi-implicit method. <i>Quart. J. R. Met. Soc.</i> , <b>101</b> , 637-655.  Forster P. M. D., Blackburn M., Glover R., Shine K. P., 2000: An examination of climate sensitivity for idealised climate change experiments in an intermediate general circulation model. <i>Climate Dynamics</i> , <b>16</b> , 833-849.
<b>Code</b>	FORTRAN
<b>Platform</b>	Linux
<b>Latest Update</b>	v3.1

### 3.1.1.3 UM

The MetOffice Unified Model (UM) is a general circulation model (GCM) designed to run either as a climate model or numerical weather processing (NWP) model. As a climate model it is run in two configurations: HadCM3 (see Turner et al., 2006) and HadAM3 (see Turner et al., 2009a). HadCM3 is a coupled atmosphere-ocean model. HadAM3 is an atmosphere only model. Both have a horizontal resolution of  $2.5^\circ \times 3.75^\circ$  and 19 vertical levels. These models are based on the 'Old Dynamics' of UM 4.5, which employs a non-linear, hydrostatic set of dynamical equations on a horizontal latitude-longitude grid. In NWP mode the model is run as a high resolution regional model, which has been run over Antarctica with a horizontal resolution of 12 km and 38 vertical levels (see Turner et al., 2009b). Lateral boundary conditions are generated by running a global model. This model is based on the 'New Dynamics' of UM 6.1, which solves nonhydrostatic, deep-atmosphere dynamics using a semi-implicit, semi-lagrangian numerical scheme. All models contain comprehensive parameterizations. HadCM3 and HadAM3 are run on the local HADES linux cluster. The regional NWP model is run on HECToR.

<b>Model</b>	UM
<b>Contact</b>	Andrew Orr - anmcr@bas.ac.uk
<b>Link</b>	<a href="http://ncas-cms.nerc.ac.uk/">http://ncas-cms.nerc.ac.uk/</a>
<b>Literature</b>	Turner J., Connolley W. M., Lachlan-Cope T. A., Marshall G. J., 2006: The performance of the Hadley Centre climate model (HADCM3) in high southern latitudes. <i>International Journal of Climatology</i> , <b>26</b> , 91-112.  Turner J., Comiso J. C., Marshall G. J., Lachlan-Cope T. A., Bracegirdle T., Maksym T., Meredith M. P., Wang Z., and Orr A., 2009: Non-annular atmospheric circulation change induced by stratospheric ozone depletion and its role in the recent increase of Antarctic sea ice extent. <i>Geophysical Research Letters</i> , <b>36</b> , doi:10.1029/2009GL037524.
<b>Code</b>	FORTRAN
<b>Platform</b>	HADES linux cluster (BAS) and HECToR (national)
<b>Version</b>	--

### 3.1.2 Chemistry and Past Climates

#### 3.1.2.1 HADAM3

HadAM3 is a grid point model and has a horizontal resolution of 2.5×3.75 degrees in latitude × longitude. This gives 96×73 grid points on the scalar (pressure, temperature and moisture) grid; the vector (wind velocity) grid is offset by 1/2 a grid box. This gives a resolution of approximately 300 km, roughly equal to T42 in a spectral model. There are 19 levels in the vertical. The timestep is 30 minutes (with three sub-timesteps per timestep in the dynamics). Near the poles, fields are fourier-filtered to prevent instabilities due to the CFL criterion.

<b>Model</b>	HadAM3
<b>Contact</b>	Louise Sime - lsime@bas.ac.uk
<b>Link</b>	--
<b>Literature</b>	Sime L. C., Tindall J. C., Wolff E. W., Connolley W. M., and Valdes P. J., 2008: Antarctic isotopic thermometer during a CO2 forced warming event. <i>J. Geophys. Res.</i> , <b>113</b> (D24), D24119
<b>Code</b>	FORTRAN
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.1.2.2 HADCM3

The Hadley Centre Coupled Model Version 3 was developed from the earlier HadCM2 model. Various improvements were applied to the 19 level atmosphere model and the 20 level ocean model and as a result the model requires no artificial flux adjustments to prevent excessive climate drift. The atmosphere and ocean exchange information once per day, heat and water fluxes being conserved ... exactly. Momentum fluxes are interpolated between atmosphere and ocean grids so are not conserved precisely, but this non-conservation is not thought to have a significant effect. The main differences from the previous HadCM2 model are a significantly more sophisticated radiation scheme; the inclusion of the direct impact of convection on momentum; and the inclusion of a new land surface scheme that includes a better representation of evaporation, freezing and melting of soil moisture. The HadCM3 model was used by the Hadley Centre to provide input for the IPCC Third Assessment Report.

<b>Model</b>	HadCM3
<b>Contact</b>	Louise Sime - lsim@bas.ac.uk
<b>Link</b>	--
<b>Literature</b>	Tindall J. C., Valdes P. J., and Sime L. C., 2009: isotopic signature of ENSO and the tropical amount effect. <i>J. Geophys. Res.</i> , <b>114</b> , D04111.  Röthlisberger R., et al., 2008: The southern hemisphere at glacial terminations: insights from the Dome C ice core. <i>Clim. Past Discuss.</i> , <b>4</b> , 761-789.
<b>Code</b>	FORTRAN
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.1.2.3 P-TOMCAT

p-TOMCAT is a massively parallel tropospheric chemistry transport model: p-TOMCAT stands for parallelised-Tropospheric Offline Model of Chemistry and Transport.

<b>Model</b>	p-TOMCAT
<b>Contact</b>	--
<b>Link</b>	<a href="http://www.atm.ch.cam.ac.uk/cas/trop-mod/trop_models.html">http://www.atm.ch.cam.ac.uk/cas/trop-mod/trop_models.html</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN 77 and 90
<b>Platform</b>	HPCx
<b>Latest Update</b>	v1.5 (2009)

### 3.1.3 Ecosystems

N/A

### 3.1.4 Environmental Change and Evolution

N/A

### 3.1.5 Ice Sheets

#### 3.1.5.1 BASISM

BASISM is an ice-sheet simulator. It operates in two modes; as a typical ice-sheet simulator (ISS mode) and as a balance velocity model (BVM mode). In ISS mode it solves the evolution equations for ice thickness, with optional thermo-mechanical coupling and the incorporation of horizontal stress gradients. In BVM mode, thickness history is prescribed, and continuity is used to determine the velocity fields. These are used to compute ice temperature and age.

<b>Model</b>	BASISM
<b>Contact</b>	Richard Hindmarsh - rcah@bas.ac.uk
<b>Link</b>	--
<b>Literature</b>	Hindmarsh R. C. A., 2001: Notes on basic glaciological computational methods and algorithms. Continuum Mechanics and Applications in Geophysics and the Environment, Springer-Verlag, Berlin Heidelberg, Germany.  Hindmarsh R. C. A., Leysinger Vieli G. J-M. C., and Parrenin F., 2009: A large-scale numerical model for computing isochrone geometry. <i>Ann. Glaciol.</i> , <b>51</b> , (in press).
<b>Code</b>	Matlab, C
<b>Platform</b>	Windows, Linux, Mac
<b>Latest Update</b>	v1.3 (2009)

#### 3.1.5.2 BERKFUN

BERKFUN computes the vertical distribution of temperature and age in the central parts of ice-sheets where horizontal flow has a negligible influence on the profiles. It contains options for time-dependent behaviour and for automatically computing the melt-rate if the ice reaches the pressure-melting point.

<b>Model</b>	BERKFUN
<b>Contact</b>	Richard Hindmarsh rcah@bas.ac.uk
<b>Link</b>	--
<b>Literature</b>	Hindmarsh, R C A., 1999: On the numerical computation of temperature in an ice-sheet. <i>J. Glaciol.</i> , <b>45</b> (151), 568-574.  Hindmarsh R. C. A., Leysinger Vieli G. J-M. C., and Parrenin F., 2009: A large-scale numerical model for computing isochrone geometry. <i>Ann. Glaciol.</i> , <b>51</b> , (in press).
<b>Code</b>	Matlab, C
<b>Platform</b>	Windows, Linux, Mac
<b>Latest Update</b>	v1.4 (2009)

### 3.1.5.3 PSISM

PSISM solves the Stokes equations to compute flow of isothermal ice sliding over rigid bedrock or deforming sediment. It uses pseudo-spectral methods to discretise the governing equations. It is intended to be used for small-scale (horizontal distances of tens of metres to tens of kilometres) process studies, and is not an ice-sheet simulator.

<b>Model</b>	PSISM
<b>Contact</b>	Richard Hindmarsh rcah@bas.ac.uk
<b>Link</b>	--
<b>Literature</b>	Pattyn F., Perichon L., Aschwanden A., Breuer B., De Smedt B., Gagliardini O., Gudmundsson G. H., Hindmarsh R. C. A., Hubbard A., Johnson J V., Kleiner T., Konovalov Y., Martin C., Payne A. J., Pollard D., Price S., Ruckamp M., Saito F., Souček O., Sugiyama S., and Zwinger T., 2008: Benchmark experiments for higher order and full-Stokes ice sheet models (ISMIP-HOM). <i>The Cryosphere</i> , <b>2</b> , 95-108.
<b>Code</b>	Matlab, C
<b>Platform</b>	Windows, Linux, Mac
<b>Latest Update</b>	v1.4 (2009)

### 3.1.6 Oceans

N/A

### 3.2 BRITISH GEOLOGICAL SURVEY

Founded in 1835, the British Geological Survey (BGS) is the nation's principal supplier of objective, impartial and up-to-date geological expertise and information for decision making for governmental, commercial and individual users. BGS carries out research in strategically important areas including energy and natural resources, vulnerability to environmental change and hazards, and Earth System Science, often in collaboration with the national and international scientific academic community. In this way BGS maintains and develops understanding of earth sciences to improve policy-making, enhance national wealth and reduce risk.

#### 3.2.1 Climate Change

N/A

#### 3.2.2 Earth Hazards and Systems

##### 3.2.2.1 BGGM

The BGGM (BGS Global Geomagnetic Model) is a spherical harmonic representation of the Earth's main magnetic field and its changes with time. Annual updating of the BGGM allows inclusion of the latest data collected from satellites and magnetic observatories around the world and any developments in the modelling techniques applied, so improving the accuracy of the model. The BGGM is widely accepted as a standard in the oil industry, for use in directional drilling with magnetometers.

<b>Model</b>	BGGM
<b>Contact</b>	Susan Macmillan - smac@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/bggm.html">http://www.geomag.bgs.ac.uk/bggm.html</a>
<b>Literature</b>	Macmillan S., 2007: Going Underground. <i>Navigation News</i> , September/October, 20-21.  Thomson A. W. P., and Lesur V., 2007: An improved geomagnetic data selection algorithm for global geomagnetic field modelling. <i>Geophysical Journal International</i> , <b>169</b> , 951-963.
<b>Code</b>	C/Java
<b>Platform</b>	inverse model – Cluster, forward model - Windows/Linux/Solaris
<b>Latest Update</b>	2009

##### 3.2.2.2 IGRF

The IGRF (International Geomagnetic Reference Field) is a spherical harmonic representation of the Earth's main magnetic field and its changes with time. It is produced by collaboration between BGS and several other institutes around the world.

<b>Model</b>	IGRF
<b>Contact</b>	Susan Macmillan - smac@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/navigation.html">http://www.geomag.bgs.ac.uk/navigation.html</a> <a href="http://www.ngdc.noaa.gov/IAGA/vmod/">http://www.ngdc.noaa.gov/IAGA/vmod/</a>
<b>Literature</b>	Macmillan S., and Maus S., 2005: International Geomagnetic Reference Field - the tenth generation. <i>Earth, Planets and Space</i> , <b>57</b> , 1135-1140.  Lesur V., Macmillan S., and Thomson A. W. P., 2005: The BGS magnetic field candidate models for the 10th generation IGRF. <i>Earth, Planets and Space</i> , <b>57</b> , 1157-1164.
<b>Code</b>	Fortran and C
<b>Platform</b>	inverse model – Cluster, forward model - Windows/Linux/Solaris
<b>Latest Update</b>	2004

### 3.2.2.3 OSMOD

The UK regional magnetic field model is a polynomial representation of the Earth's main magnetic field and its changes with time, valid for the region of the UK. It is produced by BGS and its main use is for the magnetic north service for the Ordnance Survey.

<b>Model</b>	OSMOD
<b>Contact</b>	Susan Macmillan - smac@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/gifs/gma_calc.html">http://www.geomag.bgs.ac.uk/gifs/gma_calc.html</a>
<b>Literature</b>	Shanahan T., and Macmillan S., 2008: Provision of magnetic north information to the Ordnance Survey - the 2008 annual report. British Geological Survey Commissioned Report, CR/08/164.
<b>Code</b>	Fortran
<b>Platform</b>	Solaris
<b>Latest Update</b>	2009

### 3.2.2.4 SWIMIC

SWIMIC (Solar Wind Monitoring and Induction Modelling for Geomagnetically Induced Currents) is a web page system that provides daily forecasts of geomagnetic activity, advanced warning of geomagnetic storm onset, monitoring data during storms and a model of geomagnetically induced currents (GIC) in the Scottish part of the UK power grid. Induced surface electric field estimates derived from real-time monitoring of the Earth's magnetic field are combined with a model of the conductivity of the Earth's surface and a power grid network model to predict GIC in the Scottish power grid in near real time.

<b>Model</b>	SWIMIC
<b>Contact</b>	Alan Thomson - awpt@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/gicpublic/">http://www.geomag.bgs.ac.uk/gicpublic/</a> <a href="http://www.esa-spaceweather.net/sda/swimic/">http://www.esa-spaceweather.net/sda/swimic/</a>
<b>Literature</b>	Thomson A. W. P., 2006: Light Sky at Night? Power Companies Fright! <i>Planet Earth</i> , <b>Spring</b> , 26-27.  Thomson A. W. P., McKay A. J., Clarke E., and Reay S. J. 2005: Surface electric fields and geomagnetically induced currents in the Scottish Power grid during the 30 October 2003 geomagnetic storm. <i>Space Weather</i> , <b>3</b> (S11002), 14.
<b>Code</b>	Fortran
<b>Platform</b>	Solaris
<b>Latest Update</b>	2009

### 3.2.2.5 SOLMAG AND PDFLAP

SOLMAG and PDFLAP are solar flux and magnetic index forecasting models which are real-time auto-regressive models for use in estimating upper atmospheric air density and its effect on satellite drag and geomagnetic induced currents in power grid networks. The prediction time for SOLMAG is solar cycle (11 years) and that for PDFLAP is solar rotation (27 days).

<b>Model</b>	SOLMAG/PDFLAP
<b>Contact</b>	Alan Thomson - awpt@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/gifs/forecast.html">http://www.geomag.bgs.ac.uk/gifs/forecast.html</a>
<b>Literature</b>	Thomson A.W. P., 1996: Non-linear predictions of Ap by activity class and numerical value. <i>Journal Pure and Applied Geophysics</i> , <b>146</b> (1).
<b>Code</b>	Fortran
<b>Platform</b>	Solaris
<b>Latest Update</b>	2009

### 3.2.2.6 WMM

The WMM (World Magnetic Model) is a spherical harmonic representation of the Earth's main magnetic field and its changes with time. It is produced by collaboration between the BGS and the US National Oceanic and Atmospheric Administration and is widely used in military and civilian navigation systems.

<b>Model</b>	WMM
<b>Contact</b>	Susan Macmillan - smac@bgs.ac.uk
<b>Link</b>	<a href="http://www.geomag.bgs.ac.uk/navigation.html">http://www.geomag.bgs.ac.uk/navigation.html</a> <a href="http://www.ngdc.noaa.gov/geomag/WMM/">http://www.ngdc.noaa.gov/geomag/WMM/</a>
<b>Literature</b>	McLean S., Macmillan S., Maus S., Lesur V., Thomson A. W. P., and Dater D., 2004: The US/UK World Magnetic Model for 2005-2010. NOAA Technical Report NESDIS/NGDC-1.  Macmillan S., 2005: What's behind the World Magnetic Model? <i>The Hydrographic Journal</i> , <b>117</b> , 22-23.
<b>Code</b>	Fortran, C
<b>Platform</b>	inverse model – Cluster, forward model - Windows/Linux/Solaris
<b>Latest Update</b>	2004

### 3.2.3 Energy

#### 3.2.3.1 TOUGH2

TOUGH2 is a numerical simulator for non-isothermal flows of multi-component, multiphase fluids in one, two, and three-dimensional porous and fractured media. The chief applications for which TOUGH2 is designed are; geothermal reservoir engineering, nuclear waste disposal, environmental assessment and remediation, and unsaturated and saturated zone hydrology.

<b>Model</b>	TOUGH2
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www-esd.lbl.gov/TOUGH+/manuals/TOUGH2_V2_Users_Guide.pdf">http://www-esd.lbl.gov/TOUGH+/manuals/TOUGH2_V2_Users_Guide.pdf</a>
<b>Literature</b>	Liu H-H., and Illangasekare T. H., 2008: Recent Advances in Modeling Multiphase Flow and Transport with the TOUGH Family of Codes. <i>Vadose Zone J.</i> , <b>7</b> , 284-286.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, LINUX, UNIX, Mac
<b>Latest Update</b>	v2.0 (1999)

### 3.2.4 Environmental Geoscience Baselines

N/A

### 3.2.5 Geology and Landscape UK

N/A

### 3.2.6 Groundwater Sciences

#### 3.2.6.1 BGSPT

Pumping tests are traditionally analysed using simple graphical or type-curve methods. Such techniques become impractical when more than two or three parameters have to be determined and then computer-based techniques need to be employed. BGSPT is such a computer program. It has two elements: one for analysing pumping tests (PTFIT), and the other to simulate time-drawdown behaviour for a specified set of parameters (PTSIM). The model upon which both elements are based is a well, fully-penetrating a semi-confined aquifer of infinite extent.

<b>Model</b>	BGSPT
<b>Contact</b>	David Macdonald - dmjm@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/bgspt/home.html">http://www.bgs.ac.uk/bgspt/home.html</a>
<b>Literature</b>	Kulkarni I H., Shankar P. S. V., Deolankar S. B., and Shah M., 2004: Groundwater demand management at local scale in rural areas of India: a strategy to ensure water well sustainability based on aquifer diffusivity and community participation. <i>Hydrogeology Journal</i> , <b>12</b> (2), 184-196.
<b>Code</b>	FORTRAN
<b>Platform</b>	DOS
<b>Latest Update</b>	--

#### 3.2.6.2 FEFLOW

Finite Element Flow (FEFlow) is a three dimensional, finite element, groundwater modelling software package which specialises in the representation of density dependent flow in the subsurface. It can be used in steady state or transient flow, over multiple free surfaces, in saturated or unsaturated flow situations, and for mass and heat transport simulation.

<b>Model</b>	FEFlow
<b>Contact</b>	Ann Williams - atw@bgs.ac.uk
<b>Link</b>	<a href="http://www.feflow.info/">http://www.feflow.info/</a>
<b>Literature</b>	Trefry M.G., and Muffels C., 2007: FEFLOW: a finite-element ground water flow and transport modeling tool. <i>Ground Water</i> , <b>45</b> (5), 525-528.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v5.3 (2006)

## 3.2.6.3 GW25D

A GW25D model was developed by BGS based on 2D finite-difference groundwater flow equations, to simulate 2.5D groundwater flow at the national scale. GW25D produces spatial groundwater level based on the inputs of spatial distributed recharge (or constant recharge), spatial distributed transmissivity (or constant transmissivity), river stage points, and abstraction points (optional). The format of GW25D input file is compatible with both ZOOM family of groundwater models, and GIS raster format. GW25D can be applied in small and large scales with simply data input. GW25D produces steady-state groundwater levels at the moment, and transient flow equations will be incorporated into the model to simulate the time variant groundwater level in next version.

<b>Model</b>	GW25D
<b>Contact</b>	Lei Wang - lelei@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C++
<b>Platform</b>	Windows
<b>Latest Update</b>	v2.4 (2009)

## 3.2.6.4 MODFLOW

MODFLOW is three dimensional, finite difference, groundwater flow model, which can incorporate multiple packages, simulates steady and non-steady flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to having the principal directions aligned with the grid axes), and the storage coefficient may be heterogeneous. Specified head and specified flux boundaries can be simulated as can a head dependent flux across the model's outer boundary that allows water to be supplied to a boundary block in the modelled area at a rate proportional to the current head difference between a "source" of water outside the modelled area and the boundary block.

<b>Model</b>	MODFLOW
<b>Contact</b>	Andrew Hughes - aghug@bgs.ac.uk
<b>Link</b>	<a href="http://pubs.usgs.gov/tm/2005/tm6A16/PDF/TM6A16.pdf">http://pubs.usgs.gov/tm/2005/tm6A16/PDF/TM6A16.pdf</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN 90 and C
<b>Platform</b>	Windows, LINUX, UNIX, Mac
<b>Latest Update</b>	v3.0 (2009)

### 3.2.6.5 MODPATH

MODPATH is a particle-tracking post-processing package that was developed to compute three-dimensional flow paths using output from steady-state or transient ground-water flow simulations by MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model. The particle tracking package consists of two Fortran computer codes: MODPATH, which calculates particle paths, and MODPATH-PLOT, which displays results graphically.

<b>Model</b>	MODPATH
<b>Contact</b>	Andrew Hughes - aghug@bgs.ac.uk
<b>Link</b>	<a href="http://water.usgs.gov/software/MODPATH/">http://water.usgs.gov/software/MODPATH/</a>
<b>Literature</b>	Goody D. C., Hughes A. G., Williams A. T., Armstrong A. C., Nicholson R. J., and Williams J. R., 2006: Field and modelling studies to assess the risk to UK groundwater from earth-based stores for livestock manure. <i>Soil Use and Management</i> , <b>17</b> (2), 128-137.
<b>Code</b>	FORTRAN 77 and 90
<b>Platform</b>	Windows, LINUX, UNIX, Mac
<b>Latest Update</b>	v3.2 (2000)

### 3.2.6.6 MT3D

MT3D is a comprehensive three-dimensional numerical model for simulating solute transport in complex hydrogeologic settings. MT3D has a modular design that permits simulation of transport processes independently or jointly. MT3D is capable of modelling advection in complex steady-state and transient flow fields, anisotropic dispersion, first-order decay and production reactions, and linear and nonlinear sorption. It can also handle bioplume-type reactions, monad reactions, and daughter products. This enables MT3D to do multi-species reactions and simulate or assess natural attenuation within a contaminant plume. MT3D is linked with the USGS groundwater flow simulator, MODFLOW, and is designed specifically to handle advectively-dominated transport problems without the need to construct refined models specifically for solute transport.

<b>Model</b>	MT3D
<b>Contact</b>	Andrew Hughes - aghug@bgs.ac.uk
<b>Link</b>	<a href="http://hydro.geo.ua.edu/mt3d/mt3dms_v5_supplemental.pdf">http://hydro.geo.ua.edu/mt3d/mt3dms_v5_supplemental.pdf</a>
<b>Literature</b>	Andrews C. B., and Neville C. J., 2003: Ground water flow in a desert basin: challenges of simulating transport of dissolved chromium. <i>Ground Water</i> , <b>41</b> (2), 219-226.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v5.2 (2006)

## 3.2.6.7 PHAST

PHAST simulates multi-component, reactive solute transport in three-dimensional saturated ground-water flow systems. PHAST is a versatile ground-water flow and solute-transport simulator with capabilities to model a wide range of equilibrium and kinetic geochemical reactions. The flow and transport calculations are based on a modified version of HST3D that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with the geochemical model PHREEQC, which is embedded in PHAST.

<b>Model</b>	PHAST
<b>Contact</b>	Corinna Abesser - cabe@bgs.ac.uk
<b>Link</b>	<a href="http://pubs.usgs.gov/tm/2005/tm6A8/">http://pubs.usgs.gov/tm/2005/tm6A8/</a>
<b>Literature</b>	Abesser C., 2009: Development of a geochemical transport model for the Gatehampton abstraction site using PHAST. Nottingham, UK, British Geological Survey. OR/09/005.
<b>Code</b>	--
<b>Platform</b>	Windows, Linux
<b>Latest Update</b>	v1.5.1 (2008)

## 3.2.6.8 R GWL SIMULATOR

This tool allows the user to predict groundwater levels and to hind-cast in the chalk. The tool contains a user interface with several input files where the user specifies the physical models to be used, the range of respective parameters and other options. The Monte Carlo simulation outputs the values of the parameters of the runs that meet a threshold value for the correlation or RMSE. The user can then use the values from the best model to predict groundwater levels under different rainfall scenarios that need to be provided. The model used is divided in two parts: the recharge to the surface and the storage in the saturated zone. The first can be modelled through a transfer function which distributes the recharge over a period of time. Alternatively, the effective precipitation can be passed directly to the groundwater model. The options for the later are based on the saturated zone model which allows for a distributed transmissivity and storativity with minimum and maximum values set below and above specified heads respectively

<b>Model</b>	R GWL Simulator
<b>Contact</b>	Chris Jackson - crja@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Calver A., 1997: Recharge Response Functions. <i>Hydrology and Earth System Sciences</i> , <b>1</b> , 47-53. Keating T., 1982: A Lumped Parameter Model of a Chalk Aquifer-Stream System in Hampshire, UK. <i>Ground Water</i> , <b>20</b> (4), 430-36.
<b>Code</b>	R
<b>Platform</b>	Windows, Unix, Linux, Mac
<b>Latest Update</b>	v1.31 (2009)

### 3.2.6.9 LAYERED-R- $\theta$ MODEL

The finite-difference, three dimensional, radial flow model simulates groundwater flow to analyse pumping test results. The model simulates groundwater flow in homogeneous or heterogeneous aquifers under confined or unconfined conditions. Groundwater flows in aquifers under unconfined conditions are simulated using a moving water table and a collapsing finite-difference grid technique. The model also simulates important processes taking place in the vicinity of the pumped well such as well losses and the seepage face.

<b>Model</b>	Radial Flow Model
<b>Contact</b>	Majdi Mansour - majm@bgs.ac.uk
<b>Link</b>	N/A
<b>Literature</b>	Mansour M.M., Hughes A. G. And Spink A. E.F., 2005. User manual for the layered R $\theta$ model. British Geological Survey Internal Report OR/07/029.
<b>Code</b>	C++
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.02 (2008)

### 3.2.6.10 SWIFT

SWIFT is a fully-transient, three-dimensional model to simulate groundwater flow, heat, brine and radionuclide transport in porous and fractured geologic media. The primary equations for fluid flow, heat and brine are coupled by fluid density, viscosity and porosity. In addition to transient analysis, SWIFT offers a steady-state option for coupled flow and brine. The equations are solved using central or backward spatial and time weighting approximations by the finite-difference method. In addition to Cartesian, cylindrical grids may be used. Contaminant transport includes advection, dispersion, sorption and decay, including chains of constituents. Both dual-porosity and discrete-fracture representations along with rock matrix interactions may be simulated. The nonlinearities resulting from water table and variable density are solved iteratively.

<b>Model</b>	SWIFT
<b>Contact</b>	Ann Williams - atw@bgs.ac.uk
<b>Link</b>	<a href="http://www.geotransinc.com/Swift_UsersGuide.PDF">http://www.geotransinc.com/Swift_UsersGuide.PDF</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows, LINUX, UNIX,
<b>Latest Update</b>	v2.6 (2000)

## 3.2.6.11 TOUGH2

TOUGH2 is a numerical simulator for non-isothermal flows of multi-component, multiphase fluids in one, two, and three-dimensional porous and fractured media. The chief applications for which TOUGH2 is designed are; geothermal reservoir engineering, nuclear waste disposal, environmental assessment and remediation, and unsaturated and saturated zone hydrology.

<b>Model</b>	TOUGH2
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www-esd.lbl.gov/TOUGH+/manuals/TOUGH2_V2_Users_Guide.pdf">http://www-esd.lbl.gov/TOUGH+/manuals/TOUGH2_V2_Users_Guide.pdf</a>
<b>Literature</b>	Liu H-H., and Illangasekare T. H., 2008: Recent Advances in Modeling Multiphase Flow and Transport with the TOUGH Family of Codes. <i>Vadose Zone J.</i> , <b>7</b> , 284-286.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, LINUX, UNIX, Mac
<b>Latest Update</b>	v2.0 (1999)

## 3.2.6.12 ZETUP

ZETUP is the pre-processor for the finite difference groundwater flow model ZOOMQ3D. It is used to construct the model grid, which may contain multiple areas of local grid refinement, and to create rivers within these complex meshes. ZETUP produces the input files required by ZOOMQ3D that define the structure of the model mesh and the structure of rivers. It also produces templates of all of the other files required by ZOOMQ3D in the correct format. These can subsequently be modified using a text editor to complete the model specification. Finally, it produces a set of files that enable the visualisation and checking of the model structure.

<b>Model</b>	ZETUP
<b>Contact</b>	Chris Jackson - crja@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3dmodelling/zoom.html">http://www.bgs.ac.uk/science/3dmodelling/zoom.html</a>
<b>Literature</b>	Jackson C. R., Hughes A. G., Ó Dochartaigh B. É., Robins N. S., and Peach D. W., 2005: Numerical testing of conceptual models of groundwater flow: a case study using the Dumfries Basin aquifer. <i>Scottish Journal of Geology</i> , <b>41</b> (1), 51-60.  Jackson C. R. And Spink A. E. F., 2004. User's manual for ZETUP, the set up program for the groundwater flow model ZOOMQ3D. British Geological Survey Internal Report IR/04/139.
<b>Code</b>	C++
<b>Platform</b>	DOS
<b>Latest Update</b>	v1.03 (2004)

## 3.2.6.13 ZOODRM

ZOODRM is a distributed modelling code for calculating spatial and temporal variations in groundwater recharge. The model is fully compatible with the groundwater flow model ZOOMQ3D but can be used to produce a time series of recharge for other groundwater modelling codes. The model incorporates a standard Penman-Grindley type soil moisture balance method but also includes procedures for recharge estimation in arid countries, irrigated regions and urban areas.

<b>Model</b>	ZOODRM
<b>Contact</b>	Majdi Mansour - majm@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3dmodelling/zoom.html">http://www.bgs.ac.uk/science/3dmodelling/zoom.html</a>
<b>Literature</b>	Mansour M. M., And Hughes A. G., 2004: <b>DAEM Model Inventory</b> . British Geological Survey Internal Report IR/04/150.
<b>Code</b>	C++
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.04 (2009)

## 3.2.6.14 ZOOMQ3D

ZOOMQ3D is a quasi three dimensional, finite difference, groundwater flow model that uses object-orientated techniques as its basis. It incorporates mesh refinement which aids in problems related to scale. It can incorporate; multiple layers, confined and unconfined conditions, heterogeneity, anisotropy, moving boundaries, variable hydraulic conductivity with depth, recharge, abstraction, rivers, leakage, and springs.

<b>Model</b>	ZOOMQ3D
<b>Contact</b>	Chris Jackson - crja@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3dmodelling/zoom.html">http://www.bgs.ac.uk/science/3dmodelling/zoom.html</a>
<b>Literature</b>	Jackson C. R., And Spink A. E. F., 2004: User's manual for the groundwater flow model ZOOMQ3D. British Geological Survey Internal Report IR/04/140.  Jackson C. R., Hughes A. G., Ó Dochartaigh B. É., Robins N. S., and Peach D. W., 2005: Numerical testing of conceptual models of groundwater flow: a case study using the Dumfries Basin aquifer. <i>Scottish Journal of Geology</i> , <b>41</b> (1), 51-60.
<b>Code</b>	C++ and JAVA
<b>Platform</b>	Windows and UNIX
<b>Latest Update</b>	v1.03 (2004)

## 3.2.6.15 ZOOPT

ZOOPT is a steady state, time variant, particle tracking code used in conjunction with ZOOMQ3D. Like the flow model, ZOOPT is written using an object-orientated approach. The program can track the advective movement of particles both the forwards and backwards directions enabling the rapid definition of borehole catchments, recharge and discharge areas, and the visualisation of groundwater flow fields.

<b>Model</b>	ZOOPT
<b>Contact</b>	Chris Jackson - crja@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3dmodelling/zoom.html">http://www.bgs.ac.uk/science/3dmodelling/zoom.html</a>
<b>Literature</b>	Stuart M. E., Goody D. C., Hughes A. G. and Jackson C. R., 2006: A field and modelling study to determine pesticide occurrence in a public water supply in northern England, UK. <i>Ground Water Monitoring and Remediation</i> , <b>26</b> (4), 128-136.  Jackson, C. R., 2002: Steady-state particle tracking in the object-oriented regional groundwater model ZOOMQ3D, British Geological Survey Commissioned Report CR/02/210N. Environment Agency Technical Report NC/01/38/2.
<b>Code</b>	C++
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.03 (2004)

## 3.2.6.16 ZOOM\_VIEWER

A utility program that allows the creation of river spline files to be used with the ZETUP pre-processor. This application also allows a quick visual check of the flow model ZOOMQ3D input data files. It is also used to prepare the input files of the distributed recharge model ZOODRM.

<b>Model</b>	ZOOM_Viewer
<b>Contact</b>	Majdi Mansour - majm@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3dmodelling/zoom.html">http://www.bgs.ac.uk/science/3dmodelling/zoom.html</a>
<b>Literature</b>	--
<b>Code</b>	Visual C++
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.0 (2009)

## 3.2.6.17 UNNAMED GROUNDWATER MODEL 1

This model is currently being developed and refined, and looks at sensitivity of recharge, pumping and aquifer properties on pumped nitrogen concentrations.

<b>Model</b>	Unnamed Groundwater Model 1
<b>Contact</b>	Andy Butcher - asb@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	FORTRAN, Excel
<b>Platform</b>	Windows
<b>Latest Update</b>	--

### 3.2.7 Land Use and Development

#### 3.2.7.1 PHREEQC

PHREEQC is a computer program designed to perform a wide variety of low- temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modelling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits.

<b>Model</b>	PHREEQC
<b>Contact</b>	--
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Windows, LINUX, Mac
<b>Latest Update</b>	v2.15 (2008)

#### 3.2.7.2 RWEQ

The Revised Wind Erosion eQuation (RWEQ) represents the latest developments in wind erosion prediction from research undertaken in the USA since the 1930s. The precursor to RWEQ was the original Wind Erosion Equation (WEQ). The RWEQ estimates soil eroded and transported by wind between the soil surface and a height of two metres. The RWEQ differs from WEQ in that the central factor in the former is the wind, whilst in the latter soil erodibility is the dominant component. Full model implementation uses monthly weather data, soil property data, land management inputs. For site-specific studies the latter includes detailed information on crops, tillage, dates of on-site activity, irrigation and wind barrier information. For the purpose of national-scale wind erosion estimation, many of these detailed datasets will not be available at the required spatial and temporal scales, so implementation of the full, process-based version of the model is not possible. However, it is possible to use parameters within the RWEQ model for national scale erosion assessment by estimating the distribution of monthly wind erosion

potential based on climatic factors and soil factors across the landscape. The strengths of this approach include its reliance on empirical relationships which have been widely validated and the ease with which it relates to the dominant driver of erosion, wind strength.

<b>Model</b>	RWEQ
<b>Contact</b>	Barry Rawlins- bgr@bgs.ac.uk
<b>Link</b>	<a href="http://www.csrl.ars.usda.gov/wewc/rweq/readme.htm">http://www.csrl.ars.usda.gov/wewc/rweq/readme.htm</a>
<b>Literature</b>	Fryrear, D. W., Saleh, A., Bilbro, J. D., Schomberg, H. M., Stout, J. E. and Zobeck, T. M. 1998. Revised Wind Erosion Equation. USDA Wind Erosion and Water Conservation Unit, Technical Bulletin No. 1. USDA, Texas.
<b>Code</b>	MS Dos
<b>Platform</b>	Windows
<b>Latest Update</b>	--

### 3.2.7.3 WHAM

WHAM (Windermere Humic-Aqueous Model) is designed to calculate equilibrium chemical speciation in surface and ground waters, sediments and soils. The model is especially suitable for problems where the chemical speciation is dominated by organic matter (humic substances). WHAM combines Humic Ion-Binding Model V with a simple inorganic speciation code for aqueous solutions. Precipitation of aluminium and iron oxides, cation-exchange on an idealized clay mineral, and adsorption-desorption reactions of fulvic acid are also taken into account. The importance of ion accumulation in the diffuse layers surrounding the humic molecules is emphasized. WHAM has two important limitations: the precipitation and dissolution of solids cannot be simulated and oxidation–reduction (redox) reactions cannot be simulated.

<b>Model</b>	WHAM
<b>Contact</b>	Barbara Palumbo-Roe - bpal@bgs.ac.uk
<b>Link</b>	<a href="http://windermere.ceh.ac.uk/aquatic_processes/wham/index.html">http://windermere.ceh.ac.uk/aquatic_processes/wham/index.html</a>
<b>Literature</b>	Christensen J. B., Botma J. J., and Christensen T. H., 1999: Complexation of Cu and Pb by DOC in polluted groundwater: a comparison of experimental data and predictions by computer speciation models (WHAM and MINTEQA2). <i>Water Research</i> , <b>33</b> (15), 3231-3238.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v6 (2002)

### 3.2.8 Marine Geosciences

N/A

### 3.2.9 Minerals and Waste

#### 3.2.9.1 GWB PRO

Geochemist Workbench (GWB) Professional contains tools for balancing reactions, calculating activity diagrams, computing speciation in aqueous solutions, modelling reaction processes and graphing results of such models, plus programs for modeling reactive transport in one and two dimensions, and for plotting modeling results.

<b>Model</b>	GWB PRO v6
<b>Contact</b>	Barbara Palumbo-Roe - bpal@bgs.ac.uk
<b>Link</b>	<a href="http://www.rockware.com/product/supportLobby.php?id=132">http://www.rockware.com/product/supportLobby.php?id=132</a>
<b>Literature</b>	Bethke C. M., 1996: <i>Geochemical Reaction Modeling: Concepts and Applications</i> . Oxford University Press, NY, USA.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v8 (2009)

#### 3.2.9.2 PHREEQC

PHREEQC is a computer program designed to perform a wide variety of low- temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modelling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits.

<b>Model</b>	PHREEQC
<b>Contact</b>	Barbara Palumbo-Roe - bpal@bgs.ac.uk
<b>Link</b>	<a href="http://wwwbr.cr.usgs.gov/projects/GWC_coupled/phreeqc/">http://wwwbr.cr.usgs.gov/projects/GWC_coupled/phreeqc/</a>
<b>Literature</b>	Lipson D. S., McCray J. E., and Thyne G. D., 2007: Using PHREEQC to simulate solute transport in fractured bedrock. <i>Ground Water</i> , <b>45</b> (4), 468-472.
<b>Code</b>	C
<b>Platform</b>	Windows, LINUX, Mac
<b>Latest Update</b>	v2.15 (2008)

### 3.2.9.3 WHAM

WHAM (Windermere Humic-Aqueous Model) is designed to calculate equilibrium chemical speciation in surface and ground waters, sediments and soils. The model is especially suitable for problems where the chemical speciation is dominated by organic matter (humic substances). WHAM combines Humic Ion-Binding Model V with a simple inorganic speciation code for aqueous solutions. Precipitation of aluminium and iron oxides, cation-exchange on an idealized clay mineral, and adsorption-desorption reactions of fulvic acid are also taken into account. The importance of ion accumulation in the diffuse layers surrounding the humic molecules is emphasized. WHAM has two important limitations: the precipitation and dissolution of solids cannot be simulated and oxidation–reduction (redox) reactions cannot be simulated.

<b>Model</b>	WHAM
<b>Contact</b>	Barbara Palumbo-Roe - bpal@bgs.ac.uk
<b>Link</b>	<a href="http://windermere.ceh.ac.uk/aquatic_processes/wham/index.html">http://windermere.ceh.ac.uk/aquatic_processes/wham/index.html</a>
<b>Literature</b>	Christensen J. B., Botma J. J., and Christensen T. H., 1999: Complexation of Cu and Pb by DOC in polluted groundwater: a comparison of experimental data and predictions by computer speciation models (WHAM and MINTEQA2). <i>Water Research</i> , <b>33</b> (15), 3231-3238.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v6 (2002)

## 3.2.10 Spatial Geoscience Technologies

### 3.2.10.1 ACOUSTIC LAYER

Acoustic Layer calculates transmission and reflection coefficients in the frequency-domain, and wavepacket transmission and reflection in the time-domain, for plane acoustic waves normally incident on layered media.

<b>Model</b>	Acoustic Layer
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	Mathematica
<b>Platform</b>	Any
<b>Latest Update</b>	v3 (2009)

## 3.2.10.2 AGI2MLE

Agi2mle converts resistivity data from the AGI SuperSting format to the BGS ALERT format.

<b>Model</b>	Agi2mle
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v5.85 (2008)

## 3.2.10.3 ALERT2R2D

Alert2r2d converts ALERT resistivity data to Res2DInv input format for inversion.

<b>Model</b>	Alert2r2d
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2009)

## 3.2.10.4 ARRAYOPT

ArrayOpt produces optimised Electrical Resistivity Tomography survey configurations. 2 versions exist, using different optimisation schemes (X4 and X5).

<b>Model</b>	ArrayOpt
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	vX4 and X5 (2007)

## 3.2.10.5 CSVREORDER

CSVreorder reorganises ALERT .csv format command files to minimise errors caused by electrode polarisation.

<b>Model</b>	CSVreorder
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2009)

## 3.2.10.6 FILTERS4

Filters4 applies a variety of screening and pre-processing filters to resistivity and induced polarisation data collected by the BGS ALERT system.

<b>Model</b>	Filters4
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v4 (2009)

## 3.2.10.7 GENBHELEC

Genbhelec creates cross-borehole resistivity survey designs in AGI SuperSting command format.

<b>Model</b>	Genbhelec
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2006)

## 3.2.10.8 GOCAD

Geological Object Computer Aided Design (GOCAD) facilitates the construction of realistic geologic surfaces. The surfaces are composed of triangular facets to provide maximum generality. Surfaces are constrained to fit various data (points, lines, slope, distance, other surfaces, well-markers, etc.). The surfaces are combined to form a 3D solid model that decomposes the sub-surface into 3D regions and layers. Each 3D region can be filled with properties.

<b>Model</b>	GOCAD
<b>Contact</b>	Holger Kessler - hke@bgs.ac.uk
<b>Link</b>	<a href="http://www.gocad.org/">http://www.gocad.org/</a>
<b>Literature</b>	Merritt J. E., and Whitbread K., 2007: Combining ARC GIS maps and attributed 3D geological models to provide geoscience solutions in the urban environment. Urban and Regional Data Management. Taylor & Francis Group, London.
<b>Code</b>	C++
<b>Platform</b>	HP/HP-UX, IBM/AIX, SGI/IRX, Solaris and Windows
<b>Latest Update</b>	--

## 3.2.10.9 GSI3D

Geological Surveying and Investigation in 3D (GSI3D) utilises a Digital Terrain Model, surface geological linework and downhole borehole data to enable the geologist to construct cross sections by correlating boreholes and the outcrops to produce a geological fence diagram. Mathematical interpolation between the nodes along the drawn sections and the limits of the units produces a solid model comprising a stack of triangulated objects each corresponding to one of the geological units present. Geologists draw their sections based on facts such as borehole logs correlated by intuition - the shape 'looks right' to a geologist. This 'looks right' element pulls on the geologists' wealth of understanding of earth processes, examination of exposures and theoretical knowledge gathered over a career in geology. The models are used in groundwater resource management and aquifer vulnerability assessments. The BGS is responding to the increasing need of reliable groundwater models by creating direct links between GSI3D and the groundwater modelling software ZOOMQ3D (2.2.6.14)

<b>Model</b>	GSI3D
<b>Contact</b>	Holger Kessler - hke@bgs.ac.uk
<b>Link</b>	<a href="http://www.bgs.ac.uk/science/3Dmodelling/gsi3d.html">http://www.bgs.ac.uk/science/3Dmodelling/gsi3d.html</a>
<b>Literature</b>	Kessler H., Mathers S. J., and Sobisch H-G., 2009: The capture and dissemination of integrated 3D geospatial knowledge at the British Geological Survey using GSI3D software and methodology. <i>Computers &amp; Geosciences</i> , <b>35</b> , 1311-1321.
<b>Code</b>	Java
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 3.2.10.10 RES2D/3DINV

Res2D and 3DInv are fast and flexible codes for inverting resistivity and induced polarisation data using 2.5D or 3D models respectively. Time-lapse inversion capability is available in Res2DInv.

<b>Model</b>	Res2D/3DInv
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	<a href="http://www.geoelectrical.com/index.php">http://www.geoelectrical.com/index.php</a>
<b>Literature</b>	--
<b>Code</b>	C & Assembly language (commercial, closed source)
<b>Platform</b>	Windows
<b>Latest Update</b>	3.58.35 (2D), 2.21.30 (3D) (10/09/2009)

## 3.2.10.11 STG2RES2DINV/STG2RES3DINV

Stg2res2Dinv/Stg2res3Dinv convert AGI SuperSting resistivity data to Res2D/3DInv input files for inversion.

<b>Model</b>	Stg2res2Dinv/Stg2res3Dinv
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2008)

## 3.2.10.12 STGEXTRECIP

StgExtRecip extracts reciprocal pair average measurements and associated error estimates from AGI SuperSting resistivity data.

<b>Model</b>	Stg2res2Dinv/Stg2res3Dinv
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2008)

## 3.2.10.13 SPZ

Spz calculates tomographic images of charge density probability from self-potential survey data (including data from borehole electrodes).

<b>Model</b>	Spz
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v5 (2005)

## 3.2.10.14 TIMEINTERP

Timeinterp corrects resistivity data from the BGS ALERT instrument for changes in the subsurface resistivity distribution during data acquisition.

<b>Model</b>	Timeinterp
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2007)

## 3.2.10.15 TIMELAPSE

Timelapse reformats timelapse resistivity data from the BGS ALERT instrument for processing with Res2DInv.

<b>Model</b>	Timelapse
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2007)

## 3.2.10.16 TLCOMPARE

Tlcompare analyses timelapse resistivity survey data for statistically significant changes, to decide whether inversion is worthwhile.

<b>Model</b>	Tlcompare
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	C
<b>Platform</b>	Any
<b>Latest Update</b>	v1 (2008)

## 3.2.10.17 UNCERTAINTY ESTIMATION SOFTWARE

It is thought that a dedicated Uncertainty Estimation Software system would be a good approach for documenting sources of uncertainty and a start has been made on developing software for constructing cause and effect diagrams that BGS staff will be able to use specifically for modelling applications. The system is being developed with an underlying data structure, and the graphics are generated dynamically from this data. A major advantage of this approach is that the data will be available for compiling reports and for storage in meta data tables. Graphical tools for creating these sorts of diagrams are however currently available within MS Visio, but there is no underlying metadata.

<b>Model</b>	Uncertainty Estimation Software
<b>Contact</b>	Mark Cave - mrca@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Cave M. R., and Wood B., 2002: Approaches to the Measurement of Uncertainty in Geoscience Data Modelling. BGS Internal Report IR/02/68.
<b>Code</b>	MATLAB
<b>Platform</b>	--
<b>Latest Update</b>	v1.2

## 3.2.10.18 XH\_ELEC\_POS\_ERRORS

XH\_elec\_pos\_errors calculates estimates of relative errors in measured apparent resistivity caused by uncertainties in electrode positions.

<b>Model</b>	XH_elec_pos_errors
<b>Contact</b>	Paul Wilkinson - pbw@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	Mathematica
<b>Platform</b>	Any
<b>Latest Update</b>	v3 (2007)

### 3.2.11 Other BGS Models

#### 3.2.11.1 AT123D

AT123D, analytical, transient One-, Two-, and Three-Dimensional Model, is an analytical groundwater transport model. AT123D computes the spatial-temporal concentration distribution of wastes in the aquifer system and predicts the transient spread of a contaminant plume through a groundwater aquifer. The fate and transport processes accounted for in AT123D are advection, dispersion, adsorption, and decay. AT123D estimates all the above components on a monthly basis for up to 99 years of simulation time. AT123D can be used as an assessment tool to help the user estimate the dissolved concentration of a chemical in three dimensions in groundwater resulting from a mass release over a source area. AT123D can handle: two kinds of source releases – instantaneous, continuous with a constant loading or time-varying releases; three types of waste–radioactive, chemicals, heat; four types of source configurations—a point source, a line source parallel to the x-, y-, z-axis, an area source perpendicular to the z-axis, a volume source; four variations of the aquifer dimensions–finite depth and finite width, finite depth and infinite width, infinite depth and finite width, infinite depth and infinite width.

<b>Model</b>	AT123D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.scisoftware.com/products/at123d_overview/at123d_overview.html">http://www.scisoftware.com/products/at123d_overview/at123d_overview.html</a>
<b>Literature</b>	Yeh G. T., 1981: AT123D: analytical transient one-, two-, and three-dimensional simulation of waste transport in the aquifer system. ORNL-5602. , Oak Ridge National Laboratory, Oak Ridge, TN.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	--

#### 3.2.11.2 BIOMOC

BIOMOC is a two-dimensional model that can simulate the transport and biotransformation of multiple reacting solutes. The program is general and flexible, allowing for any combination of biodegradation processes. A number of expressions for biological transformation rates have been included as options in the code. These include single, multiple, and minimum Monod kinetics and competitive, noncompetitive, and Haldane inhibition. The kinetic parameters can be formulated to simulate zero-order or first-order approximations of biodegradation rates. The

growth and decay of several microbial populations performing the transformations is also accounted for. The microbial growth can be disabled, limited by biomass inhibition, or limited by the availability of a specified nutrient.

<b>Model</b>	BIOMOC
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://water.usgs.gov/software/biomoc.html">http://water.usgs.gov/software/biomoc.html</a>
<b>Literature</b>	Essaid H. I., and Bekins B. A., 1997: BIOMOC, A multispecies solute-transport model with biodegradation: U.S. Geological Survey Water-Resources Investigations Report 97-4022.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, DOS, UNIX
<b>Latest Update</b>	v1.0 (1999)

### 3.2.11.3 BIOSCREEN

BIOSCREEN is a screening model which simulates remediation through natural attenuation of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions that have been shown to be the dominant biodegradation processes at many petroleum release sites. Includes three different model types: (1) solute transport without decay, (2) solute transport with biodegradation modeled as a first-order decay process (simple, lumped-parameter approach), and (3) solute transport with biodegradation modeled as an instantaneous biodegradation reaction with multiple soluble electron acceptors including dissolved oxygen, nitrate, and sulfate. The model is designed to simulate biodegradation by both aerobic and anaerobic reactions.

<b>Model</b>	BIOSCREEN
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.epa.gov/ada/csmos/models/bioscrn.html#System">http://www.epa.gov/ada/csmos/models/bioscrn.html#System</a>
<b>Literature</b>	Karanovic M., Neville C. J., and Andrews C. B., 2007: BIOSCREEN-AT: BIOSCREEN with an Exact Analytical Solution. <i>Ground Water</i> , <b>45</b> (2), 242-245.
<b>Code</b>	Excel
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.4 (1997)

## 3.2.11.4 CHAIN2D

CHAIN\_2D is a model for simulating two-dimensional variably saturated water flow, heat transport, and the movement of solutes involved in sequential first-order decay reactions. The program numerically solves the Richards' equation for saturated-unsaturated water flow and the convection-dispersion equation for solute and heat transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The water flow part of the model can deal with prescribed head, gradient, and flux boundaries, as well as boundaries controlled by atmospheric conditions. Free drainage boundary condition and a simplified representation of nodal drains using results of electric analog experiments is also included. The heat transport equation considers transport due to conduction and convection with flowing water. The solute transport equations consider convective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equation includes provisions for nonlinear nonequilibrium reactions between the solid and the liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions.

<b>Model</b>	CHAIN2D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.ars.usda.gov/Services/docs.htm?docid=8914">http://www.ars.usda.gov/Services/docs.htm?docid=8914</a>
<b>Literature</b>	Simunek J., and van Genuchten M Th., 1994: The CHAIN_2D code for simulating the two-dimensional movement of water, heat, and multiple solutes in variably saturated porous media, Version 1.1. Research Report No. 136, 194 p., U.S. Salinity Laboratory, USDA, ARS, Riverside, California.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	--
<b>Latest Update</b>	v1.0 (1984)

## 3.2.11.5 COLUMN2

COLUMN2 is a 1 dimensional computer program designed for studies of the effects of various physicochemical processes on migration. It solves the solute transport equation and can take into account dispersion, sorption, ion exchange, first and second order homogeneous chemical reactions. Spatial variations of input pulses and retention factors are possible. The method of solution is based on a finite difference discretization followed by the application of the method of characteristics and two separate grid systems.

<b>Model</b>	COLUMN2
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.risoe.dk/rispubl/reports_INIS/RISOR514.pdf">http://www.risoe.dk/rispubl/reports_INIS/RISOR514.pdf</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN 77
<b>Platform</b>	--
<b>Latest Update</b>	v1.0 (1984)

## 3.2.11.6 CXTFIT

CXTFIT estimates solute transport parameters using a nonlinear least-squares parameter optimization method. The program may be used to solve the inverse problem by fitting mathematical solutions of theoretical transport models, based upon the convection-dispersion equation (CDE), to experimental results. This approach allows parameters in the transport models to be quantified. The program may also be used to solve the direct or forward problem to determine the concentration as a function of time and /or position. Three different one-dimensional transport models are included: (i) the conventional CDE; (ii) the chemical and physical nonequilibrium CDE; and (iii) a stochastic stream tube model based upon the local-scale CDE with equilibrium or nonequilibrium adsorption. The two independent stochastic parameters in the stream-tube model are the pore water velocity, and either the dispersion coefficient, the distribution coefficient, or the nonequilibrium rate parameter. These pairs of stochastic parameters are described with a bivariate lognormal probability density function.

<b>Model</b>	CXTFIT
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.ars.usda.gov/Services/docs.htm?docid=8915">http://www.ars.usda.gov/Services/docs.htm?docid=8915</a>
<b>Literature</b>	Toride N., Leij F. J., and van Genuchten M. Th., 1995: The CXTFIT Code for Estimating Transport Parameters from Laboratory or Field Tracer Experiments, Version 2.0. Research Report No. 137, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	--
<b>Latest Update</b>	v2.0 (1995)

## 3.2.11.7 FATMIC

FATMIC 2D (2DFATMIC) and FATMIC 3D (3DFATMIC) simulate subsurface flow, transport, and fate of contaminants which are undergoing chemical and/or biological transformations. The model is applicable to transient conditions in both saturated and unsaturated zones. The flow module is a Galerkin finite element solution of Richard's equation. The transport module is a hybrid Lagrangian-Eulerian approach with an adapted zooming and peak capturing algorithm. This model can almost eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective transport.

<b>Model</b>	FATMIC
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.epa.gov/ada/csmos/models/3dfatmic.html">http://www.epa.gov/ada/csmos/models/3dfatmic.html</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	UNIX
<b>Latest Update</b>	v1.0 (1997)

## 3.2.11.8 FLUVSIM

FLUVSIM simulates sediment accumulation at the channel belt/floodplain scale producing sedimentologic and stratigraphic attributes that it converts to petrophysical properties for groundwater modeling. The three-dimensional distribution of attributes results from self-organized critical behaviour of the stratigraphic process-response system given spatial and temporal variation of the accommodation space and sediment supply ratio (A/S), which is analogous to base level. Process parameter functions driving base-level variation include the rate of sea (or lake) level change, regional subsidence rate, and water and sediment flux into the model.

<b>Model</b>	FLUVSIM
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://inside.mines.edu/~epoeter/research/FluvSim/index.shtml">http://inside.mines.edu/~epoeter/research/FluvSim/index.shtml</a>
<b>Literature</b>	Deutsch C. V., and Tran T. T., 2002: FLUVSIM: a program for object-based stochastic modeling of fluvial depositional systems. <i>Computers &amp; Geosciences</i> , <b>28</b> (4), 525-535.
<b>Code</b>	FORTRAN, C++
<b>Platform</b>	Mac
<b>Latest Update</b>	--

## 3.2.11.9 FTRANS

FTRANS (Fractured flow and Transport of RAdioNuclideS) is a two-dimensional finite-element code designed to simulate ground-water flow and transport of radioactive nuclides in a fractured porous return medium. FTRANS takes into account fluid interactions between the fractures and porous matrix blocks, advective-dispersive transport in the fractures and diffusion in the porous matrix blocks, and chain reactions of radionuclide components. It has the capability to model the fractured system using either the dual-porosity or the discrete- fracture modeling approach or a combination of both. FTRANS can be used to perform two-dimensional near-field or far-field predictive analyses of ground-water flow and to perform risk assessments of radionuclide transport from nuclear waste repository subsystems to the biosphere.

<b>Model</b>	FTRANS
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Hölttä P., Siitari-Kauppi M., Hakanen M., and Tukiainen V., 2001: Attempt to model laboratory-scale diffusion and retardation data. <i>Journal of Contaminant Hydrology</i> , <b>47</b> (2-4), 139-148.
<b>Code</b>	FORTRAN4
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.2.11.10 HTS3D

The Heat- and Solute-Transport Program (HST3D) simulates ground-water flow and associated heat and solute transport in three dimensions. Over the years since the release of Versions 1.0 through 1.4, various additions, modifications, and corrections have been made to the original simulator. Major changes included in Version 2 are (1) a revised data-input file with all spatial information described by coordinate location; (2) a new iterative solver for the matrix equations based on a generalized conjugate-gradient method; (3) an evapotranspiration boundary condition; (4) a division of the simulator output into many files; (5) a new set of output files designed for use by post-processing programs for graphical visualization and for flow totalisation; (6) a pre-processor for evaluating dimensioning requirements; and (7) a post-processor for totalizing boundary flow rates and cumulative amounts. The post-processing program for graphical visualization must be supplied by the user. Version 2 of the simulator has been verified using five test problems selected from the published literature. One involves heat transport, four involve solute transport, and all have variable-density fluids.

<b>Model</b>	HST3D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://wwwbrr.cr.usgs.gov/projects/GW_Solute/hst/">http://wwwbrr.cr.usgs.gov/projects/GW_Solute/hst/</a>
<b>Literature</b>	Bravo H. R., Jiang F., and Hunt R. J., 2002: Using groundwater temperature data to constrain parameter estimation in a groundwater flow model of a wetland system. <i>Water Resources Research</i> , 38(8), 28-1, 28-14.
<b>Code</b>	FORTRAN 90
<b>Platform</b>	Windows, Linux, Unix
<b>Latest Update</b>	v2.2.13 (2006)

## 3.2.11.11 HYDRAQL

HYDRAQL is a programme for the computation of chemical equilibrium composition of aqueous batch systems including surface complexation modelling of ion adsorption at the oxide/solution interface.

<b>Model</b>	HYDRAQL
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Muurinen A., and Lehtikoinen J., 1999: Porewater chemistry in compacted bentonite. <i>Engineering Geology</i> , 54(1-2), 207-214.
<b>Code</b>	--
<b>Platform</b>	Mac
<b>Latest Update</b>	--

## 3.2.11.12 HYDROTHERM

Quantitative modeling of magmatic-hydrothermal systems has been hampered by the lack of publicly available models for multiphase, high-temperature flow. The HYDROTHERM model described here is a finite-difference model for three-dimensional, multiphase flow of pure water and heat over a temperature range of 0 to 1,200 degrees Celsius and a pressure range of 0.5 to 10,000 bars. HYDROTHERM solves numerical approximations to mass- and energy-balance equations that are posed in terms of pressure and enthalpy. Major assumptions are that the rock matrix can be treated as a porous medium; that water and rock are in thermal equilibrium; and that capillary pressure is negligible. HYDROTHERM allows one- and two-dimensional radial simulations as well as one-, two-, and three-dimensional simulations in Cartesian coordinates. The program structure is modular to allow easy modification.

<b>Model</b>	HYDROTHERM
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.wr.usgs.gov/projects/GW_Solute/hydrotherm/">http://www.wr.usgs.gov/projects/GW_Solute/hydrotherm/</a>
<b>Literature</b>	Ingebritsen S. E., and Hayba D. O., 1994: Fluid flow and heat transport near the critical point of water: <i>Geophysical Research Letters</i> , <b>21</b> , 2199-2202.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, LINUX
<b>Latest Update</b>	v3.1 (2008)

## 3.2.11.13 HYDRUS-1D

HYDRUS is a computer model designed to simulate one-dimensional water flow, single-species solute transport, and heat movement, in variably-saturated porous media. The program numerically solves the Richards' equation for saturated-unsaturated water flow and Fickian-based advection dispersion equations for heat and solute transport. The Flow equation incorporates a sink term to account for water uptake by plant roots. The Heat transport equation considers conduction as well as convection with flowing water. The Solute transport equations consider advective-dispersive transport in the liquid phase, and diffusion in the gaseous phase. The transport equations also include provisions for: Nonlinear and/or Nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero order production, and two First-order degradation reactions: One which is independent of other solutes, and one which provides the coupling between solutes involved in sequential first-order decay reactions. The program may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media.

<b>Model</b>	HYDRUS-1D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.pc-progress.com/en/Default.aspx?H1D-description#k1">http://www.pc-progress.com/en/Default.aspx?H1D-description#k1</a>
<b>Literature</b>	Hilten R. N., Lawrence T. M., and Tollner E. W., 2008: Modeling stormwater runoff from green roofs with HYDRUS-1D. <i>Journal of Hydrology</i> , <b>358</b> (3-4), 288-293.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v6.0 (2009)

## 3.2.11.14 MECOSIM

MECOSIM is a one dimensional transport code for mecoprop (an organic pollutant) with degradation by Monod kinetics

<b>Model</b>	MECOSIM
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.2.11.15 MINEQL

MINEQL is a powerful and easy-to-use chemical equilibrium modeling system that can be used to perform calculations on low temperature (0-50oC), low to moderate ionic strength (<0.5 M) aqueous systems. MINEQL+ is a data driven program, so you do NO programming. In the simplest scenario, you create systems by selecting chemical components from a menu, scan the thermodynamic database and run the calculation. However, MINEQL+ also provides tools to allow you to take control of your reaction data, create a personal thermodynamic database, perform synthetic titrations and automatically process mutiple samples (such as field data).

<b>Model</b>	MINEQL
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.mineql.com/">http://www.mineql.com/</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v4.6 (2007)

## 3.2.11.16 MT3DMS

MT3DMS is a modular three-dimensional transport model that can simulate advection, dispersion, and chemical reactions of dissolved constituents. MT3DMS uses the output head and cell-by-cell flow data computed by MODFLOW to establish the groundwater flow field. GMS supports both pre-processing and post-processing with MT3DMS. As with MODFLOW, GMS provides several "packages" which simplify user-input. This data is then used by MT3DMS when MT3DMS is run, and the solution can then be read back into GMS for visualization. GMS has the ability to produce film loops and .avi animations as shown below. MT3DMS has the capability of modelling changes in concentrations of groundwater contaminants due to advection, dispersion, diffusion, and some chemical reactions including equilibrium-controlled linear or non-linear sorption, and first-order irreversible or reversible kinetic reactions.

<b>Model</b>	MT3DMS
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.xmswiki.com/xms/GMS:MT3DMS">http://www.xmswiki.com/xms/GMS:MT3DMS</a> <a href="http://www.geology.wisc.edu/courses/g727/mt3dmanual.pdf">http://www.geology.wisc.edu/courses/g727/mt3dmanual.pdf</a>
<b>Literature</b>	Hecht-Mendez J., Molina-Giraldo N., Bayer P., and Blum P., 2009: Heat transport modelling using the multi-species transport model MT3DMS. <i>Geophysical Research Abstracts</i> , <b>11</b> , EGU2009-12030, 2009. EGU General Assembly 2009.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v5.20 (2006)

### 3.2.11.17 NAPL (2D/3D)

NAPL Simulator conducts a simulation of the contamination of soils and aquifers which results from the release of organic liquids commonly referred to as Non-Aqueous Phase Liquids (NAPLS). The simulator is applicable to three interrelated zones: a vadose zone which is in contact with the atmosphere, a capillary zone, and a water-table aquifer zone. Three mobile phases are accommodated: water, NAPL, and gas. The 3-phase k-S-P sub-model accommodates capillary and fluid entrapment hysteresis. NAPL dissolution and volatilization are accounted for through rate-limited mass transfer sub-models.

<b>Model</b>	NAPL (2D/3D)
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.epa.gov/ada/csmos/models/napl.html">http://www.epa.gov/ada/csmos/models/napl.html</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	DOS, Unix
<b>Latest Update</b>	v1.0 (1997)

### 3.2.11.18 POLF

A finite-element program for modelling two-dimensional (2D) pollutant transport in confined and unconfined aquifers is presented. The code accounts for the absorption and biological decay of the pollutant, which is supposed to behave as a tracer. The flow and pollutant transport equations are solved by using either a Galerkin finite-element (GFE) or a control-volume finite-element (CVFE) formulation. The discretisation of the flow domain is obtained by using triangular finite elements and linear shape functions, whereas integration in time is performed by a finite-difference (FD) Picard scheme. For two problems of which the analytical solution is known, the results of the simulations carried out by the CVFE and by GFE formulations are compared, taking as evaluation parameters the global mass-balance errors and the average deviation between the numerical and analytical solutions.

<b>Model</b>	POLF
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Gottardi G., 1998: POLF: Two-dimensional finite-element model for predicting the areal flow of pollutant in confined and unconfined aquifers. <i>Computers and Geosciences</i> , 26(6), 509-522.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	--
<b>Latest Update</b>	--

### 3.2.11.19 RT3D

RT3D is a multi-species reactive transport model developed by the Battelle Pacific Northwest National Laboratory. RT3D is a modified version of MT3DMS that utilises alternate Chemical Reaction packages. Numerous pre-defined reactions are available and an option is provided for creating user-defined reactions. RT3D is well-suited for simulating natural attenuation and bioremediation.

<b>Model</b>	RT3D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.xmswiki.com/xms/GMS:RT3D">http://www.xmswiki.com/xms/GMS:RT3D</a>
<b>Literature</b>	Johnson C. D., and Truex M. J., 2006: RT3D Reaction Modules for Natural and Enhanced Attenuation of Chloroethanes, Chloroethenes, Chloromethanes, and Daughter Products. Pacific Northwest National Laboratory, US Department of Energy, Washington, USA.
<b>Code</b>	FORTRAN90
<b>Platform</b>	Windows, UNIX
<b>Latest Update</b>	v2.5 (2003)

### 3.2.11.20 SEAWAT-2000

SEAWAT-2000 is a previous release of the SEAWAT computer program for simulation of three-dimensional, variable-density, transient ground-water flow in porous media. SEAWAT-2000 was designed by combining a modified version of MODFLOW-2000 and MT3DMS into a single computer program. The code was developed using the MODFLOW-2000 concept of a process, which is defined as “part of the code that solves a fundamental equation by a specified numerical method.” SEAWAT-2000 contains all of the processes distributed with MODFLOW-2000 and also includes the Variable-Density Flow Process (as an alternative to the constant-density Ground-Water Flow Process) and the Integrated MT3DMS Transport Process. Processes may be active or inactive, depending on simulation objectives; however, not all processes are compatible. For example, the Sensitivity and Parameter Estimation Processes are not compatible with the Variable-Density Flow and Integrated MT3DMS Transport Processes. The SEAWAT-2000 computer code was tested with the common variable-density benchmark problems and also with problems representing evaporation from a salt lake and rotation of immiscible fluids.

<b>Model</b>	SEAWAT
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://water.usgs.gov/ogw/seawat/summary2k.html">http://water.usgs.gov/ogw/seawat/summary2k.html</a>
<b>Literature</b>	Al-Maktoumi A., Lockington D. A., and Volker R. E., 2007: SEAWAT 2000: modelling unstable flow and sensitivity to discretization levels and numerical schemes. <i>Hydrogeology Journal</i> , <b>15</b> (6), 1119-1129.
<b>Code</b>	FORTRAN 77/90
<b>Platform</b>	Windows, DOS
<b>Latest Update</b>	v3.13 (2006)

### 3.2.11.21 SEEP2D

SEEP2D is a two-dimensional finite element groundwater model designed to be used on profile models (XZ models) such as cross-sections of earth dams or levees. SEEP2D can be used for either confined or unconfined steady state flow models. For unconfined models, there are two options for determining the phreatic surface. With the first option, the mesh is automatically truncated as the iterative solution process proceeds and when the model converges, the upper boundary of the mesh corresponds to the phreatic surface. With the second option, both saturated and unsaturated flow is simulated and the mesh is not modified. The phreatic surface can be displayed by turning on the phreatic surface option in the display options dialog.

<b>Model</b>	SEEP2D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.xmswiki.com/xms/GMS:SEEP2D">http://www.xmswiki.com/xms/GMS:SEEP2D</a> <a href="http://www.seepage-analysis.com/html/seep2d.html">http://www.seepage-analysis.com/html/seep2d.html</a>
<b>Literature</b>	Zee C-H., and Zee R., 2006: Earthquake Hydrodynamic Pressure on Dams. <i>J. Hydr. Engrg.</i> , <b>132</b> (11), 1128-1133.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows
<b>Latest Update</b>	v5

### 3.2.11.22 STAFAN

STATistical Fault ANalysis (STAFAN) is proposed as an alternative to fault simulation of digital circuits. In this analysis, controllability and observability of circuit nodes are defined as probabilities which are estimated from signal statistics obtained from fault-free simulation. Special procedures are developed for dealing with these quantities at fanout nodes and at feedback nodes. The computed probabilities are used to derive unbiased estimates of fault detection probabilities and overall fault coverage for the given set of input vectors. Fault coverage and the undetected fault data obtained from STAFAN for actual circuits are shown to agree favorably with the fault simulator results. The computational complexity added to a fault-free simulator by STAFAN grows only linearly with the number of circuit nodes.

<b>Model</b>	STAFAN
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

### 3.2.11.23 SUPCRT

SUPCRT (an abbreviation for "supercritical") is a package for calculating the standard molal thermodynamic properties of aqueous, gaseous, liquid and crystalline mineral and organic species and reactions between them from 1 to 5000 bar and 0 to 1000 °C.

<b>Model</b>	SUPCRT
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.predcent.org/download/supcrt">http://www.predcent.org/download/supcrt</a>
<b>Literature</b>	Johnson J. W., Oelkers E. H., and Helgeson H. C., 1992: SUPCRT92: A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bar and 0 to 1000°C. <i>Comp. Geosci.</i> , <b>18</b> , 899-947.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, DOS
<b>Latest Update</b>	--

### 3.2.11.24 SUTRA\_MS

A modified version of SUTRA is introduced that is capable of simulating variable-density flow and transport of heat and multiple dissolved species through variably to fully saturated porous media. The original version of SUTRA is capable of simulating variable-density flow and transport of either heat or one dissolved species through variably to fully saturated porous media. This modified version was developed because of the importance of temperature and solute concentrations in many variable-density flow environments and the desire to implicitly simulate the transport of multiple dissolved species that may or may not affect fluid density. Users familiar with SUTRA should have little difficulty applying this version of SUTRA to multi-species transport problems.

<b>Model</b>	SUTRA_MS
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://water.usgs.gov/nrp/gwsoftware/sutra.html">http://water.usgs.gov/nrp/gwsoftware/sutra.html</a> <a href="http://pubs.usgs.gov/of/2004/1207/pdf/OFR2004-1207web.pdf">http://pubs.usgs.gov/of/2004/1207/pdf/OFR2004-1207web.pdf</a>
<b>Literature</b>	Hughes J. D., and Sanford W. E., 2004: SUTRA-MS: A Version of SUTRA Modified to Simulate Heat and Multiple-Solute Transport: U.S. Geological Survey Open-File Report 2004-1207, 141.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v2004.1 (2004)

### 3.2.11.25 SWMS (2D/3D)

SWMS is a computer program for simulating water and solute movement in two or three dimensional variably saturated media. The program numerically solves the Richards' equation for saturated-unsaturated water flow and the convection-dispersion equation for solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The transport equation includes provisions for linear equilibrium adsorption, zero-order production, and first-order degradation. The program may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media.

<b>Model</b>	SWMS
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://igwmc.mines.edu/zipfiles/swms2.htm">http://igwmc.mines.edu/zipfiles/swms2.htm</a>
<b>Literature</b>	Simunek. J., Vogel T., van Genuchten M.Th., 1994. The SWMS_2D code for simulating water flow and solute transport in two-dimensional variably saturated media, Version 1.21. Research Report No. 132, 197 p., U.S. Salinity Laboratory, USDA, ARS, Riverside, California.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.21 (1994)

### 3.2.11.26 THERMIC

THERMIC solves the 2-dimensional (pseudo 3D for axi-symmetric cases) conductive and advective heat-transfer equation. THERMIC uses a finite-element method that takes into account realistic geometries, heterogeneous material properties and various boundary and initial conditions. As it also allows for latent heat (heat production due to crystallisation) and for thermal properties, such as thermal conductivity, to be dependent on temperature, it is particularly suited to heat transfer problems encountered in the Earth Sciences.

<b>Model</b>	THERMIC
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	--
<b>Literature</b>	Bonneville A., and Capolsini P., 1999: THERMIC: a 2-D finite-element tool to solve conductive and advective heat transfer problems in Earth Sciences. <i>Computers and Geosciences</i> , <b>25</b> (10), 1137-1148.
<b>Code</b>	C
<b>Platform</b>	Windows, UNIX, SUN, SGI
<b>Latest Update</b>	--

### 3.2.11.27 TRANS1D

TRANS1D is a one dimensional solute transport code using numerical inversion of Laplace Transform solutions.

<b>Model</b>	TRANS1D
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	-
<b>Literature</b>	Khandelwal A., Rabideau A. J., Shen P., 1998: Analysis of diffusion and sorption of organic solutes in soil/bentonite barrier walls. <i>Environmental Science &amp; Technology</i> , <b>32</b> (9), 1333-1339.
<b>Code</b>	Excel
<b>Platform</b>	Windows
<b>Latest Update</b>	v3.0 (1999)

### 3.2.11.28 TRIANGLE

A Two-Dimensional Quality Mesh Generator and Delaunay Triangulator. Delaunay triangulations maximize the minimum angle of all the angles of the triangles in the triangulation; they tend to avoid skinny triangles. TRIANGLE generates exact Delaunay triangulations, constrained Delaunay triangulations, conforming Delaunay triangulations, Voronoi diagrams, and high-quality triangular meshes. The latter can be generated with no small or large angles, and are thus suitable for finite element analysis.

<b>Model</b>	TRIANGLE
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.cs.cmu.edu/~quake/triangle.html">http://www.cs.cmu.edu/~quake/triangle.html</a>
<b>Literature</b>	Shewchuk J. R., 2002: Delaunay Refinement Algorithms for Triangular Mesh Generation. <i>Computational Geometry: Theory and Applications</i> <b>22</b> (1-3), 21-74.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v1.6 (2005)

## 3.2.11.29 TRIPM

TRIPM is a mathematical model designed to predict the transport of radionuclides and their decay products in a saturated-unsaturated vertical plane of a phreatic aquifer under isothermal conditions. The model is composed of two modules: the first calculates the pressure distribution in the domain of interest, enabling one to compute the velocities and soil moistures; the second calculates the migration of the various species by taking into account the major processes associated with the transport phenomena of a dissolved substance in porous media, i.e. advection, mechanical dispersion, molecular diffusion, radio- active decay and sorption. The influence of soil-water pH on the distribution coefficient is also considered.

<b>Model</b>	TRIPM
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.nea.fr/abs/html/nesc1028.html">http://www.nea.fr/abs/html/nesc1028.html</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.2.11.30 UNSAT-H

UNSAT-H uses a finite-difference approximation to solve the one-dimensional vertical form of Richard's equation, which governs unsaturated moisture movement. UNSAT-H was designed for use in water balance studies and has capabilities to estimate evaporation resulting from meteorological surface conditions and transpiration from plants. Parameters required for each material type are saturated hydraulic conductivity ( $K_s$ , cm/hr), volumetric moisture content at saturation ( $\theta_s$ ), irreducible moisture content ( $\theta_r$ ), air entry head ( $h_e$ , cm H<sub>2</sub>O), and inverse pore size distribution index ( $b$ ). A site-specific curve was developed for the existing soil based on laboratory samples. Predicting the future long-term performance of low-level wastes at any near-surface burial site in terms of migration of contaminants requires a model capable of simulating water flow in the unsaturated soils above the buried waste. UNSAT-H is also used to simulate the effects of various practices to enhance isolation of wastes.

<b>Model</b>	UNSAT-H
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://ecobas.org/www-server/rem/mdb/unsat-h.html">http://ecobas.org/www-server/rem/mdb/unsat-h.html</a>
<b>Literature</b>	Khire M. V., Benson C. H., and Bosscher P. J., 1999: Field Data from a Capillary Barrier and Model Predictions with UNSAT-H. <i>Journal of Geotechnical and Geoenvironmental Engineering</i> , <b>125</b> (6), 518-527.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	Windows, Unix
<b>Latest Update</b>	v3.0 (2000)

## 3.2.11.31 UTCHEM

Application: Originally a three-dimensional finite difference model for multiphase flow, transport and chemical flooding, the UTCHEM code has been modified to transform it into a general purpose NAPL simulator. Appropriate physical, chemical and biological process models have been incorporated into the simulator to create a 3D multiphase multi-component model capable of simulating the fate and transport of NAPL's in the saturated and unsaturated zones of aquifers. The model can be used to simulate the actual field operation of remediation activities such as surfactant remediation or bioremediation as well as laboratory experiments with large-scale aquifer models.

<b>Model</b>	UTCHEM
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://www.epa.gov/ada/csmos/models/utchem.html#Installation">http://www.epa.gov/ada/csmos/models/utchem.html#Installation</a>
<b>Literature</b>	Jawitz J. W., Annable M. D., and Rao P.S.C., 1998: Miscible fluid displacement stability in unconfined porous media: Two-dimensional flow experiments and simulations. <i>Journal of Contaminant Hydrology</i> , <b>31</b> (3-4), 211-230.
<b>Code</b>	FORTRAN 90
<b>Platform</b>	Windows, UNIX
<b>Latest Update</b>	v6.1 (1999)

## 3.2.11.32 WATEQ4

WATEQ4F is a chemical speciation code for natural waters. It uses field measurements of temperature, pH, Eh, dissolved oxygen and alkalinity, and the chemical analysis of a water sample as input and calculates the distribution of aqueous species, ion activities, and mineral saturation indices that indicate the tendency of a water to dissolve or precipitate a set of minerals. The model assumes homogeneous aqueous phase equilibria, except for redox species. Equilibrium with respect to mineral solubilities is not assumed. The program results are used primarily to examine the tendency of water to reach mineral solubility equilibria as a constraint on interpreting the chemistry of natural waters.

<b>Model</b>	WATEQ4
<b>Contact</b>	David Noy - djn@bgs.ac.uk
<b>Link</b>	<a href="http://wwwbrr.cr.usgs.gov/projects/GWC_chemtherm/software.htm">http://wwwbrr.cr.usgs.gov/projects/GWC_chemtherm/software.htm</a>
<b>Literature</b>	Ball J. W., and Nordstrom D. K., 1992: Geochemical model to calculate speciation of major, trace and redox elements in natural waters. International Groundwater Modelling Center, U.S. Geological Survey.
<b>Code</b>	FORTRAN 95
<b>Platform</b>	--
<b>Latest Update</b>	v2.63 (2004)

### 3.3 CENTRE FOR ECOLOGY AND HYDROLOGY

The Centre for Ecology & Hydrology (CEH) delivers independent research, survey, training and knowledge transfer in the environmental sciences to advance knowledge of planet Earth as a complex, interacting system. Located at sites in England, Scotland and Wales, their National Capability and extensive network of long-term monitoring and experimental field sites provide access to diverse ecosystems and support an internationally renowned research capacity. Their research is aimed at improving understanding of the environment and the processes that support life on Earth. They are particularly interested in the impacts of human activity on the world around us and in developing ready-to-use approaches for achieving environmental sustainability.

#### 3.3.1.1 BASFOR

BASic FORest (BASFOR) models forest biogeochemistry.

<b>Model</b>	BASFOR
<b>Contact</b>	Marcel van Oijen - mvano@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Van Oijen M., Rougier J., and Smith R., 2005: Bayesian calibration of process-based forest models: bridging the gap between models and data. <i>Tree Physiology</i> , <b>25</b> , 915-927.
<b>Code</b>	MATLAB
<b>Platform</b>	Windows, LINUX, Mac
<b>Latest Update</b>	v10

#### 3.3.1.2 BASGRA

The BASic GRAssland model (BASGRA) is used to simulate grassland growth in summer and winter.

<b>Model</b>	BASGRA
<b>Contact</b>	Marcel van Oijen - mvano@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Van Oijen M., Höglind M., Hanslin H. M., and Caldwell N., 2005: Process-based modelling of timothy regrowth. <i>Agronomy Journal</i> , <b>97</b> , 1295-1303.
<b>Code</b>	MATLAB
<b>Platform</b>	Windows, LINUX, Mac
<b>Latest Update</b>	--

## 3.3.1.3 CAF2007

The Coffee AgroForestry model 2007 (CAF2007) simulates competition between coffee and shade trees for light, nitrogen, and water.

<b>Model</b>	CAF2007
<b>Contact</b>	Marcel van Oijen - mvano@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Van Oijen M., Dauzat J., Harmand J-M., Lawson G., and Vaast P., 2009: Process-based modelling of coffee agroforestry systems in Central America: A review of quantitative information on underlying processes and development of a simple model. <i>Agroforestry Systems</i> (Submitted).
<b>Code</b>	MATLAB
<b>Platform</b>	Windows, LINUX, Mac
<b>Latest Update</b>	--

## 3.3.1.4 CASCADE-N

The Catchment Scale Delivery model - Nitrate model (CASCADE-N) is a spatially distributed water quality model operating at a spatial resolution of the HRU (hydrological response unit): a hydrologically independent unit derived by 50m DTM typically of approx 5 km<sup>2</sup>. Soils are represented using the HOST classification from which hydrological, physical and chemical parameters are derived. Soil hydrology is represented by a layer model comprising two storages (near surface and subsurface). Calibration of soil hydrology is required and can be carried out at sub-catchment or whole-catchment scale. At HRU resolution the model requires monthly values of hydrologically available soil nitrate for a range of landuses defined by combining landcover map and agricultural census data. These inputs include atmospheric deposition and additions of fertiliser and manure. For arable crops, a simplified representation of the soil N cycle is included in an Excel spreadsheet. Livestock data are used to determine the amounts of available N arising from agricultural grasslands and managed manure additions to arable land.

<b>Model</b>	CASCADE-N
<b>Contact</b>	Mike Hutchins - mihu@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Hutchins M. G., Deflandre A., and Boorman D. B., 2006: Performance benchmarking linked diffuse and in-stream water quality models. <i>Archiv fur Hydrobiologie Supplement</i> , 161. <i>Large Rivers</i> , 17, 133-154.
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 3.3.1.5 CFLOW

The Carbon FLOWs model (CFLOW) is a box-flow model for forests. Calculation of GHG fluxes associated with afforestation can be undertaken.

<b>Model</b>	CFLOW
<b>Contact</b>	Marcel van Oijen - mvano@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Milne R., and Van Oijen M., 2005: A comparison of two modelling studies of environmental effects on carbon stocks across Europe. <i>Annals of Forest Science</i> , <b>62</b> , 1-13.
<b>Code</b>	Matlab, SIMULINK
<b>Platform</b>	Windows
<b>Latest Update</b>	

## 3.3.1.6 CLASSIC

The semi-distributed continuous simulation rainfall-runoff model, CLASSIC, (Climate and Land-use Scenario Simulation In Catchments), was originally developed for estimating impacts of climate and land use change in large catchments on flood frequency. It has been further developed to be suitable for simulation across the flow range though with the emphasis on medium to high flows.

The model is applied on a grid square framework and comprises three main modules (soil water balance, drainage and channel routing), plus one optional one (snowmelt). The model has a grid to outlet structure in which the simulated runoff from each grid square is routed directly to the catchment outlet rather than through successive grids. Calibration is semi-automatic requiring percentages of six land use types and HOST classes for each grid, with physiographic information on hill-slope, altitude and the channel network derived from a DTM. Climatic inputs of rainfall, PE and temperature (for the snow module) are required for each grid square with flow data for the outlet point for final calibration. The grid square size is chosen to be appropriate for the catchment area and the variation of climatic and physiographic conditions within the catchment.

<b>Model</b>	CLASSIC
<b>Contact</b>	Sue Crooks - smcr@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Crooks, S.M. and Naden, P.S. 2007. CLASSIC: a semi-distributed modelling system. <i>Hydrology &amp; Earth System Sciences</i> , 11(1), 516-531.
<b>Code</b>	FORTTRAN
<b>Platform</b>	UNIX
<b>Latest Update</b>	2008

## 3.3.1.7 CHUM\_AM

The Chemistry of Uplands Model (CHUM\_AM) simulates acidification and heavy metal retention and transport.

<b>Model</b>	CHUM_AM
<b>Contact</b>	Edward Tipping - et@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Tipping E., Lawlor A. J., and Lofts S., 2006: Simulating the long-term chemistry of an upland UK catchment: major solutes and acidification. <i>Environ. Pollut.</i> , <b>141</b> , 151-166.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.3.1.8 DRIED-UP

DRIED-UP is set of multilevel linear regression models which link river flow, physical habitat (via information from River Habitat Survey) and the LIFE score, an index derived from macroinvertebrate community data.

<b>Model</b>	DRIED-UP
<b>Contact</b>	Mike Dunbar - mdu@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Dunbar M. J., and Mould D. J., 2008: DRIED-UP 2; Distinguishing the Relative Importance of Environmental Data Underpinning flow Pressure Assessment. Report to EA, Water Resources.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.3.1.9 DyDOC

The Dynamic DOC (DyDOC) model is a multi-horizon soil carbon cycling model that includes water and DOC transport.

<b>Model</b>	DyDOC
<b>Contact</b>	Edward Tipping - et@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Tipping E., Smith E. J., Bryant C. L., and Adamson J. K., 2007: The organic carbon dynamics of a moorland catchment in NW England. <i>Biogeochem.</i> <b>84</b> , 171-189.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v4 (2009)

## 3.3.1.10 ERICA

The ERICATool is a computerised, flexible software system that has a structure based upon the ERICA Integrated Approach to assessing the radiological risk to biota. The Tool guides the user through the assessment process, recording information and decisions and allowing the necessary calculations to be performed to estimate risks to selected animals and plants. Tier 1 assessments are media concentration based and use pre-calculated environmental media concentration limits to estimate risk quotients. Tier 2 calculates dose rates but allows the user to examine and edit most of the parameters used in the calculation including concentration ratios, distribution coefficients, percentage dry weight soil or sediment, dose conversion coefficients, radiation weighting factors and occupancy factors. Tier 3 offers the same flexibility as Tier 2 but allows the option to run the assessment probabilistically if the underlying parameter probability distribution functions are defined. Results from the Tool can be put into context using incorporated data on dose effects relationships and background dose rates.

<b>Model</b>	ERICA
<b>Contact</b>	Nick Beresford - nab@ceh.ac.uk
<b>Link</b>	<a href="http://www.ceh.ac.uk/protect/ERICAdeliverables.html">http://www.ceh.ac.uk/protect/ERICAdeliverables.html</a>
<b>Literature</b>	Special issue of Journal of Environmental Radioactivity. Volume 99, 9, September 2008
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.0 (2008)

## 3.3.1.11 FRAME

The Fine Resolution Atmospheric Multi-pollutant Exchange (FRAME) model is a Lagrangian atmospheric transport model used to assess the long-term annual mean deposition of reduced and oxidised nitrogen and sulphur as well as base cations and heavy metals over the United Kingdom. It simulates the emissions, vertical diffusion, chemical transformation in the atmosphere and deposition to vegetation by precipitation and by turbulent dry deposition of pollutants. The model runs on a number of different horizontal resolutions including 50 km over Europe and 5 km and 1 km over the UK. It is used to calculate exceedance of critical loads for acid deposition and nitrogen deposition. FRAME has been applied to support UK government policy on future emissions control of pollutants and in assessing historical deposition.

<b>Model</b>	FRAME
<b>Contact</b>	Tony Dore - todo@ceh.ac.uk
<b>Link</b>	<a href="http://www.frame.ceh.ac.uk/description.htm">http://www.frame.ceh.ac.uk/description.htm</a>
<b>Literature</b>	Dore A. J., Vieno M., Tang Y. S., Dragosits U., Dosio A., Weston K. J., Sutton M. A., 2007: Modelling the atmospheric transport and deposition of sulphur and nitrogen over the United Kingdom and assessment of the influence of SO <sub>2</sub> emissions from international shipping. <i>Atmospheric Environment</i> , <b>41</b> (11). 2355-2367.
<b>Code</b>	High Performance FORTRAN
<b>Platform</b>	Linux
<b>Latest Update</b>	V7.1 (2009)

## 3.3.1.12 GWAVA

The Global Water Availability Assessment (GWAVA) model operates at the half degree resolution i.e. approximately cells of 55km x 55km but it has also been applied successfully at 0.1 degree resolution in Bangladesh. Each grid cell operates as a single rainfall-runoff model which estimates runoff generation local to that cell; cells are linked in a way which simulates the natural drainage network and flows are accumulated through the network. Imposed within the runoff network are the water resources components such as abstractions, returns, inter-basin transfers and storage schemes etc. in a way that variations in demand both seasonally and in times of water stress are represented in a realistic manner. Demands are estimated on a cell by cell basis for each major sector: domestic water supply, industrial and agricultural. Observed daily or monthly streamflow data are required for calibration. Different types of water availability indices are calculated within GWAVA which range from a simple ratio of annual supply to demand to more complex measures which take account of seasonal variations in demand i.e. irrigation.

<b>Model</b>	GWAVA
<b>Contact</b>	Sonja Folwell - ssf@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Meigh J.R., McKenzie A. A., and Sene K. J., 1999: A grid-based approach to water scarcity estimates for eastern and southern Africa. <i>Water Resources Management</i> , <b>13</b> , 85-115.
<b>Code</b>	FORTRAN
<b>Platform</b>	UNIX
<b>Latest Update</b>	v5

## 3.3.1.13 IHDM

The Institute of Hydrology Distributed Model (IHDM) is a two dimensional hill-slope hydrological model solving Richards' equation using finite elements. Parameters up-scaled from standard core-scale soil properties.

<b>Model</b>	IHDM
<b>Contact</b>	Lisa Stuart - ejs@ceh.ac.uk
<b>Link</b>	<a href="http://nora.nerc.ac.uk/5977/1/IH_098.pdf">http://nora.nerc.ac.uk/5977/1/IH_098.pdf</a>
<b>Literature</b>	Karvonen T., Koivusalo H., Jauhiainen M., Palko J., and Wepling K., 1999: A hydrological model for predicting runoff from different land use areas. <i>Journal of Hydrology</i> , <b>217</b> (3-4), 253-265.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.3.1.14 IHMS

The Integrated Hydrological Modelling System (IHMS) comprises three models combined but can also run separately. This system is designed to represent the way the integrated water management should work i.e. the impact of change in climate, change in land use and change in abstraction on stream/river flows, drainage flow, groundwater flow, piezometric heads and seawater intrusion (only in coastal areas). The system has the advantage of being able to incorporate different scenarios of possible climate change and land use impact on surface water (streams/river), groundwater/ drainage and seawater intrusion. The System comprises three packages: DiCaSM, MODFLOW (96 and 2000) and SWI models. The Distributed Catchment scale model DiCaSM, produces the recharge data that are used as input to the groundwater flow model of the US Geological Survey, MODFLOW.

<b>Model</b>	IHMS
<b>Contact</b>	Ragab Ragab - rag@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Ragab R., and Bromley J., 2010: <i>Hydro. Processes</i> (accepted)
<b>Code</b>	V Basic
<b>Platform</b>	Windows
<b>Latest Update</b>	October 2009

## 3.3.1.15 JULES

At the core of the Joint UK Land Environment Simulator (JULES) is a model of the surface energy balance (with related fluxes such as evaporation and radiation) and a model of soil heat and moisture status. Plant and soil carbon are also simulated, and there is a dynamic vegetation (sub-) model (TRIFFID), which models competition between plant types. There are options as to how various processes, e.g. runoff generation, are described. More recent developments (not yet an official release) have focussed on "biogeochemistry", including the ECOSSE model of soil C and N, and a new vegetation model (ED). JULES can be run for a single "point" (e.g. a plot) or for a grid, with gridbox sizes from ~1km to 100s km. The computing requirements vary considerably across this range of applications and depending on run length, from a minute on a single CPU to days or weeks on a cluster.

<b>Model</b>	JULES
<b>Contact</b>	Douglas Clark - dbcl@ceh.ac.uk
<b>Link</b>	<a href="http://www.jchmr.org/jules">http://www.jchmr.org/jules</a>
<b>Literature</b>	Mercado L. M., Huntingford C., Gash J. H. C., Cox P. M., Jogireddy V., 2007: Improving the representation of radiation interception and photosynthesis for climate model applications. <i>Tellus B</i> , <b>59</b> (3). 553-565.
<b>Code</b>	FORTRAN
<b>Platform</b>	UNIX/LINUX
<b>Latest Update</b>	v2.1 (2009)

## 3.3.1.16 LANDSCAPE EVAPORATION MODEL

The purpose of the Landscape Evaporation Model is to provide time series of the spatial distributions of evaporation. It uses the Penman-Monteith and the Shuttleworth-Wallace (developed from the former) models to calculate the evaporation from a number of land cover types (each of which can have multiple types defined by differences in the parameter sets). Interception losses are handled explicitly using the adapted Gash model. The water balance is maintained by using a soil water sub-model and vertical drainage and horizontal flow are represented simply. Spatial variability is represented by a square grid. Each cell can have a different soil type and the different land cover types are tiled within each cell. The time step is not explicit but should not be sub-daily.

<b>Model</b>	Landscape Evaporation Model
<b>Contact</b>	Jon Finch - jon@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Finch J. W., 2001: Estimating change in direct groundwater recharge using a spatially distributed soil water balance model. <i>Quarterly Journal of Engineering Geology and Hydrogeology</i> , <b>34</b> : 71-83.
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows
<b>Latest Update</b>	v3.0

## 3.3.1.17 LF2000-WQX

The Low Flow 2000 Water Quality Extension (LF2000-WQX) uses river flow stats and location and quality of STW effluent discharges, it estimates the water quality (mean, SD, 90th percentile) of any river stretch in England and Wales. Can model any determinand in the WIMS database or "new" determinands. Determinands can be conservative or degradable (first order). Also can set parameters to model removal of a "new" determinand in STWs.

<b>Model</b>	LF2000-WQX
<b>Contact</b>	Richard Williams - rjw@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Williams R. J., Keller V. D. J., Johnson A. C., Young A.R., Holmes M. G. R., and Wells C., 2009: A National Risk Assessment for Intersex in Fish Arising from Steroid Estrogens. <i>Environmental Toxicology and Chemistry</i> , <b>28</b> (1), 220-230.
<b>Code</b>	Visual Basic
<b>Platform</b>	Windows
<b>Latest Update</b>	v1.01 (2009)

## 3.3.1.18 OPENMI

The Open Modelling Interface (OpenMI) can be described at two levels. At the user level, OpenMI provides a standard interface, which allows models to exchange data with each other and other modelling tools on a time step by time step basis as they run. It thus facilitates the modelling of process interactions. The models may come from different suppliers, represent processes from different domains, be based on different concepts, have different spatial and temporal resolutions and have different spatial representations including no spatial representation. A useful analogy is to consider the OpenMI as the modelling equivalent of a USB cable. At the IT level, OpenMI standard is a software component interface definition for the computational core (the engine) of the computational models in the water domain. Model components that comply with this standard can, without any programming, be configured to exchange data during computation (at run-time). This means that combined systems can be created, based on OpenMI-compliant models from different providers, thus enabling the modeller to use those models that are best suited to a particular project.

<b>Model</b>	OpenMI
<b>Contact</b>	Rodger Moore - rvm@ceh.ac.uk
<b>Link</b>	<a href="http://www.OpenMI.org">www.OpenMI.org</a>
<b>Literature</b>	Gregersen J. B., Gijssbers P. J. A., and Westen S. J. P., 2007: OpenMI : Open Modelling Interface. <i>Journal of Hydroinformatics</i> , <b>9</b> (3), 175-191.
<b>Code</b>	Java, C#
<b>Platform</b>	--
<b>Latest Update</b>	v1.4 (2009)

## 3.3.1.19 PEARLS

PEARLS (Prediction of acidification and recovery at landscape scale) was conceptualised much as CASCADE, with GIS-defined drainage units linked to a schematic stream network. The scale of conceptualisation is user-defined. The water quality status of drainage is assumed to follow a probability distribution according to a small number of landscape classes defined spatially from national databases. Downstream water quality was originally estimated by mixing, using Monte Carlo simulation. Some in-stream modelling capability has recently been developed. This is akin to QUESTOR and the instream component of CASCADE.

<b>Model</b>	PEARLS
<b>Contact</b>	David Cooper - cooper@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Evans C. D., Cooper D. M., and Gannon B., 2004: A Novel Method for Mapping Critical Loads Across a River Network: Application to the River Dart, Southwest England. <i>Water, Air, &amp; Soil Pollution: Focus</i> , 1(1-2), 437-453.
<b>Code</b>	FORTTRAN
<b>Platform</b>	Windows
<b>Latest Update</b>	v1 (2009)

## 3.3.1.20 PROTECH

PROTECH (Phytoplankton Responses to Environmental Change) simulates the dynamic responses of up to eight species of phytoplankton to environmental variability in lakes and reservoirs. PROTECH models were developed originally to fulfil a commercial, decision-support role in the management of industrial water quality, where plankton growth is an issue. The progressive refinements to the model nevertheless have a robust ecological basis. This makes PROTECH a promising tool for researching plankton community ecology. The model calculates exponents describing growth and attrition, from a base of the maximum growth rates of algal species in culture. Subject to defined thresholds, growth integrates variability in the fluxes of light and nutrients. The paper develops this philosophy and its embodiment into the structure of the model. Examples of its authenticated, validated and sensitivity-tested outputs are presented.

<b>Model</b>	PROTECH
<b>Contact</b>	Alex Elliott - alexe@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Reynolds C. S., Irish A. E., and Elliott J. A., 2001: The ecological basis for simulating phytoplankton responses to environmental change (PROTECH). <i>Ecological Modelling</i> , <b>140</b> , 271-291.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 3.3.1.21 QUESTOR

QUESTOR (Quality Evaluation and Simulation Tool for River Systems) represents a river as a series of river reaches within which physical, chemical and biological processes operate. The determinands and processes modelled are not fixed within the QUESTOR modelling environment, but are tailored to the particular application. QUESTOR is based on the earlier in-stream water quality models IHQM (Institute of Hydrology water Quality Model) and QUASAR (Quality Simulation Along Rivers). QUASAR was sold commercially for both VAX and PC systems, and is now available free of charge, but unsupported, as PC-QUASAR. The model formulation of the "basic" version of QUESTOR corresponds broadly with QUASAR.

<b>Model</b>	QUESTOR
<b>Contact</b>	David Borman - dbb@ceh.ac.uk
<b>Link</b>	<a href="http://www.ceh.ac.uk/products/software/documents/questorguidenew.pdf">http://www.ceh.ac.uk/products/software/documents/questorguidenew.pdf</a>
<b>Literature</b>	Boorman D. B., 2003: LOIS In-stream Water Quality Modelling. Part 1: Catchments and Methods. <i>Science of the Total Environment</i> , <b>314-316</b> , 335-378.
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows, UNIX
<b>Latest Update</b>	--

## 3.3.1.22 ReFH

The Revitalised Flood Hydrograph (ReFH) model is a new lumped conceptual rainfall-runoff model that has been developed for modelling flood events as a direct replacement for the Flood Studies Report rainfall-runoff method. The full ReFH flood modelling software package supports all aspects of the ReFH methods including import, storage and retrieval of observed hydrometric data. The software can be linked to most standard database systems, thereby providing the opportunity to build up a structured archive of observed flood events collected from different studies.

<b>Model</b>	ReFH
<b>Contact</b>	Thomas Kjeldsen - trkj@ceh.ac.uk
<b>Link</b>	<a href="http://www.hydrosolutions.co.uk/refh.html">http://www.hydrosolutions.co.uk/refh.html</a> <a href="http://www.ceh.ac.uk/feh2/FEHReFH.html">http://www.ceh.ac.uk/feh2/FEHReFH.html</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 3.3.1.23 RIVPACS

RIVPACS (River Invertebrate Prediction and Classification System) offers site-specific predictions of the macro-invertebrate fauna to be expected in UK river sites in the absence of major environmental stress. An expected fauna is derived from RIVPACS using environmental predictor variables. The observed fauna is sampled using standard protocols. Comparison between the observed and the expected fauna provides an assessment of site quality.

<b>Model</b>	RIVPACS
<b>Contact</b>	John Davy-Bowker --
<b>Link</b>	<a href="http://www.ceh.ac.uk/products/software/RIVPACS.html">http://www.ceh.ac.uk/products/software/RIVPACS.html</a>
<b>Literature</b>	Wright J F, Sutcliffe D W and Furse M T (Eds.) (2000) Assessing the biological quality of fresh waters: RIVPACS and other techniques. Freshwater Biological Association, Ambleside, UK.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 3.3.1.24 SCAMP

The SCAMP (Surface Chemistry Assemblage Model for Particles) model represents an attempt to derive a more generally applicable model for metal distributions. The model comprises a set of mechanistic submodels for metal binding to oxides, to natural organic matter (humic substances) and to clay. Binding to oxides is simulated using a surface complexation model, to humic substances using a discrete-site/electrostatic model, and to clay using a Donnan model for cation exchange. The model has been parameterised by drawing upon the substantial body of information in the literature on the binding of metals to isolated or synthesised oxides, clays and natural organic matter. When applying the model to natural solid-solution systems, information on the chemical composition of both the solid and solution phases must be input; the model then calculates a full chemical speciation of the system, and computes the solid-solution distributions of metals from this information.

<b>Model</b>	SCAMP
<b>Contact</b>	Edward Tipping - et@ceh.ac.uk
<b>Link</b>	--
<b>Literature</b>	Almas A. R., Lofts S., Mulder J., and Tipping E., 2007: Solubility of major cations and Cu, Zn and Cd in soil extracts of some contaminated agricultural soils near a zinc smelter in Norway: modelling with a multi-surface extension of WHAM. <i>European Journal of Soil Science</i> , <b>58</b> , 1074-1086.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 3.3.1.25 WHAM

WHAM is a chemical equilibrium speciation model for waters, including soil porewaters. Given total concentrations of ionic chemicals (e.g. major ions such as sodium and chloride, trace elements such as copper and zinc) it will predict the concentrations of the different forms (species) of each chemical at thermodynamic equilibrium. A distinctive feature of the model is that it includes the interactions of ionic chemicals with humic substances, which comprise the major part of natural organic matter in waters. These interactions can be very important in controlling pH and the chemical speciation of trace elements.

<b>Model</b>	WHAM
<b>Contact</b>	Edward Tipping - et@ceh.ac.uk
<b>Link</b>	<a href="http://windermere.ceh.ac.uk/Aquatic_Processes/WHAM">http://windermere.ceh.ac.uk/Aquatic_Processes/WHAM</a>
<b>Literature</b>	Bryan S., Tipping E., and Hamilton-Taylor J., 2004: Testing Models of Chemical Speciation in Freshwaters. <i>Environmental Geochemistry and Health</i> , <b>21</b> (4), 305-310.
<b>Code</b>	--
<b>Platform</b>	Windows
<b>Latest Update</b>	v6 (2002)

### 3.4 PROUDMAN OCEANOGRAPHIC LABORATORY

The Proudman Oceanographic Laboratory (POL) is a fully-owned research laboratory focused on research into; physics of estuarine, coastal, and shelf sea circulation; wind wave dynamics and sediment transport processes; global sea level science and geodetic oceanography; and marine technology & operational oceanography. The oceans directly affect our planet's climate and ecosystems. They are all undergoing massive changes; we need to discover and understand more about them.

#### 3.4.1.1 FVCOM

FVCOM is a prognostic, unstructured-grid, finite-volume, free-surface, 3-D primitive equation coastal ocean circulation model developed by UMASSD-WHOI joint efforts. The model consists of momentum, continuity, temperature, salinity and density equations and is closed physically and mathematically using turbulence closure submodels. The horizontal grid is comprised of unstructured triangular cells and the irregular bottom is presented using generalized terrain-following coordinates. The General Ocean Turbulent Model (GOTM) has been added to FVCOM to provide optional vertical turbulent closure schemes. FVCOM is solved numerically by a second-order accurate discrete flux calculation in the integral form of the governing equations over an unstructured triangular grid. This approach combines the best features of finite-element methods (grid flexibility) and finite-difference methods (numerical efficiency and code simplicity) and provides a much better numerical representation of both local and global momentum, mass, salt, heat, and tracer conservation. The ability of FVCOM to accurately solve scalar conservation equations in addition to the topological flexibility provided by unstructured meshes and the simplicity of the coding structure has made FVCOM ideally suited for many coastal and interdisciplinary scientific applications.

<b>Model</b>	FVCOM
<b>Contact</b>	Jiuxing Xing - <a href="mailto:jxx@pol.ac.uk">jxx@pol.ac.uk</a>
<b>Link</b>	<a href="http://fvcom.smast.umassd.edu/FVCOM/index.html">http://fvcom.smast.umassd.edu/FVCOM/index.html</a>
<b>Literature</b>	Cowles G. W., 2008: Parallelization of the FVCOM Coastal Ocean Model. <i>International Journal of High Performance Computing Applications</i> , <b>22</b> (2), 177-193.
<b>Code</b>	--
<b>Platform</b>	Linux
<b>Latest Update</b>	--

#### 3.4.1.2 FOAM

The FOAM (Forecasting Ocean Assimilation Model) system consists of the following components; physical ocean model, sea ice model, data assimilation scheme, observation processing system (quality control). The FOAM system has recently been transitioned to use the NEMO ocean model code. This is a community model that has a wide user and developer base particularly in Europe. It is used for operational short-term and seasonal forecasting and climate modelling. It will form the ocean model component of the Met Office seasonal forecasting and climate modelling systems in the near future. The sea ice component is currently modelled using the 2nd version of the Louvain-le-Neuve (LIM2) model. This has viscous-plastic dynamics (and a 3-layer thermodynamic model. This will be transitioned to use the Los Alamos CICE sea-ice model in summer 2009. This includes elastic-viscous-plastic dynamics and the possibility of using multi-layer thermodynamics and multiple ice thickness categories.

<b>Model</b>	FOAM
<b>Contact</b>	--
<b>Link</b>	<a href="http://www.ncof.co.uk/FOAM-Model-Description.html">http://www.ncof.co.uk/FOAM-Model-Description.html</a>
<b>Literature</b>	Bell M. J., Barciela R., Hines A., Martin M., Sellar A., and Storkey D., 2006: Ocean Weather Forecasting. Chapter 15: The Forecasting Ocean Assimilation Model (Foam) System. Springer Netherlands, NL.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

### 3.4.1.3 ICOM

The Imperial College Ocean Model (ICOM) is based on a number of leading-edge numerical technologies which make it unique in the world today. ICOM operates flexibly in complex 3D domains, is fully parallelised, and solves for non-hydrostatic ocean dynamics using control volume finite element discretisation methods. Importantly the computational meshes ICOM uses may be unstructured in 3D and may also adapt to optimally resolve evolving solution dynamics. In collaboration with partners at the University of Oxford, the National Oceanography Centre and the Proudman Oceanographic Laboratory, ICOM is currently being developed as an open source community model for the UK.

<b>Model</b>	ICOM
<b>Contact</b>	Philip Hall - phh@pol.ac.uk
<b>Link</b>	<a href="http://amcg.ese.ic.ac.uk/index.php?title=ICOM#Ocean_Modelling_with_ICOM">http://amcg.ese.ic.ac.uk/index.php?title=ICOM#Ocean_Modelling_with_ICOM</a>
<b>Literature</b>	Ford R., Pain C. C., Piggott M. D., 2004: A nonhydrostatic finite-element model for three-dimensional stratified oceanic flows. Part I: model formulation. <i>Monthly Weather Review</i> , <b>132</b> , 2816 - 2831.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

### 3.4.1.4 MITGCM

The MITGCM (MIT General Circulation Model) is a numerical model designed for study of the atmosphere, ocean, and climate. Its non-hydrostatic formulation enables it to simulate fluid phenomena over a wide range of scales; its adjoint capability enables it to be applied to parameter and state estimation problems. By employing fluid isomorphisms, one hydrodynamical kernel can be used to simulate flow in both the atmosphere and ocean.

<b>Model</b>	MITGCM
<b>Contact</b>	Jiuxing Xing - jxx@pol.ac.uk
<b>Link</b>	<a href="http://mitgcm.org/">http://mitgcm.org/</a> <a href="http://mitgcm.org/r2_manual/latest/online_documents/manual.pdf">http://mitgcm.org/r2_manual/latest/online_documents/manual.pdf</a>
<b>Literature</b>	Marotzke J., Giering R., Zhang K.Q., Stammer D., Hill C., and Lee T., 1999: Construction of the adjoint MIT ocean general circulation model and application to Atlantic heat transport variability. <i>J. Geophysical Res.</i> , <b>104</b> (C12), 29529-29547.
<b>Code</b>	FORTRAN 77
<b>Platform</b>	LINUX
<b>Latest Update</b>	--

#### 3.4.1.5 MOM

The GFDL Modular Ocean Model (MOM) is a three dimensional primitive equation ocean model based on the pioneering work of Kirk Bryan (1969). The original objective of this development was to build a tool for numerical modeling of the large-scale (basin-wide or global) ocean circulation using then-current algorithms based upon decomposition of the ocean into rectangular boxes of variable size, and the use of low-order finite differences approximations.

<b>Model</b>	MOM
<b>Contact</b>	Miguel Maqueda --
<b>Link</b>	<a href="http://www.gfdl.noaa.gov/ocean-model">http://www.gfdl.noaa.gov/ocean-model</a>
<b>Literature</b>	Haidvogel D. B., and Beckmann A., 1999: Numerical ocean circulation modelling. Imperial Collage Press, London, UK.
<b>Code</b>	FORTRAN 90
<b>Platform</b>	--
<b>Latest Update</b>	v4.1 (2009)

#### 3.4.1.6 NEMO

Nucleus for European Modelling of the Ocean (NEMO) is an ocean modelling framework which is composed of "engines" nested in an "environment". The "engines" provide numerical solutions of ocean, sea-ice, tracers and biochemistry equations and their related physics. The "environment" consists of the pre- and post-processing tools, the interface to the other components of the Earth System, the user interface, the computer dependent functions and the documentation of the system. NEMO allows several ocean related components of the earth system to work together or separately. It also allows a two-way nesting via the AGRIF software. It is interfaced with the remaining component of the earth system (atmosphere, land surfaces, etc) via the OASIS coupler.

<b>Model</b>	NEMO
<b>Contact</b>	Jason Holt - jholt@pol.ac.uk
<b>Link</b>	<a href="http://www.nemo-ocean.eu/">http://www.nemo-ocean.eu/</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v3.1 (2008)

#### 3.4.1.7 OCCAM 2D

The OCCAM model is based on the Bryan-Cox-Semtner ocean general circulation model. Bryan developed the initial version of the model but Semtner and Cox made important contributions which helped its rapid acceptance by the oceanographic community. The model is based on the ocean primitive equations; its main difference from other ocean models is the use of an Arakawa-B grid in the horizontal and level surfaces in the vertical. The model is in wide use by the oceanographic community, the most popular version currently being the MOM code.

<b>Model</b>	OCCAM 2D
<b>Contact</b>	Christopher Hughes - cwh@pol.ac.uk
<b>Link</b>	<a href="ftp://ftp.soc.soton.ac.uk/pub/occam/papers/occam_tech1.pdf">ftp://ftp.soc.soton.ac.uk/pub/occam/papers/occam_tech1.pdf</a>
<b>Literature</b>	Humphries, U.W. and Webb, D.J.,2008: On the Indonesian Throughflow in the OCCAM 1/4 degree ocean model. <i>Ocean Science</i> , <b>4</b> , 183-198.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

#### 3.4.1.8 POLCOMS

The Proudman Oceanographic Laboratory Coastal-Ocean Modelling System (POLCOMS) has been developed to incorporate features suitable for the modelling of baroclinic processes on the shelf, at the shelf-slope and in ocean regions to allow long term coupled ocean-shelf simulations. It includes a sophisticated advection scheme, the 'Piecewise Parabolic Method' (PPM) which gives it excellent feature-preserving properties. It is ideal for simulating on-shelf baroclinic features such as river plumes and fronts, and the transport of tracers. Moreover, the model is formulated on an Arakawa B-grid, in contrast to the C-grid used in many shelf sea models, which makes it well suited to modelling horizontal density variations.

<b>Model</b>	POLCOMS
<b>Contact</b>	Jason Holt - jholt@pol.ac.uk
<b>Link</b>	<a href="http://cobs.pol.ac.uk/modl/metfcst/POLCOMS_DOCUMENTATION/">http://cobs.pol.ac.uk/modl/metfcst/POLCOMS_DOCUMENTATION/</a>
<b>Literature</b>	Holt J. T., and James I. D., 2001: An s coordinate density evolving model of the northwest European continental shelf. 1, Model description and density structure. <i>Journal of Geophysical Research</i> , <b>106</b> , 14015-14034.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

#### 3.4.1.9 QUODDY

The Quoddy model is a full 3D baroclinic finite element model. It was modified to model the shallow water equations, retaining the main characteristic of the Quoddy model, which are: equal order of approximation for velocity and elevation, the divergence of the vertically integrated momentum equations can be recast by using the mass balance equation and eliminating the divergence of the vertically integrated mass flux. This yields a prognostic equation for the elevation of second order in time (a wave equation). Solving numerically for the three equations (two momentum equations and one wave equation) is easy and leads to a stable model, but, does not balance mass locally. To guaranty a better local conservation of mass, a weighted mass equation is added to the wave equation (the mass equation can also be viewed as a penalty term).

<b>Model</b>	QUODDY
<b>Contact</b>	Philip Hall - phh@pol.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

#### 3.4.1.10 ROMS

The Regional Ocean Model System (Roms) is a free-surface, hydrostatic, primitive equation ocean model that uses stretched, terrain-following coordinates in the vertical and orthogonal curvilinear coordinates in the horizontal. Initially, it was based on the S-coordinate Rutgers University Model (SCRUM) described by Song and Haidvogel (1994). Roms was completely rewritten to improve both its numerics and efficiency in single and multi-threaded computer architectures. It also was expanded to include a variety of new features including high-order advection schemes; accurate pressure gradient algorithms; several subgrid-scale parameterizations; atmospheric, oceanic, and benthic boundary layers; biological modules; radiation boundary conditions; and data assimilation.

<b>Model</b>	ROMS
<b>Contact</b>	Miguel Maqeda --
<b>Link</b>	<a href="http://www.myroms.org/">http://www.myroms.org/</a>
<b>Literature</b>	Chua B. S., and Bennett A. F., 2001: An Inverse Ocean Modelling System. <i>Ocean Modelling</i> , <b>3</b> , 137-165.
<b>Code</b>	FORTAN 90/95, C
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v3.2 (2009)

#### 3.4.1.11 TELEMATAC

The TELEMATAC system, which was developed at EDF/LNH, is a powerful integrated modelling tool for use in the field of free-surface flows. Having been used in the context of very many studies throughout the world (several hundred to date), it has become one of the major standards in its field. The various simulation modules use high-capacity algorithms based on the finite-element method. Space is discretised in the form of an unstructured grid of triangular elements, which means that it can be refined particularly in areas of special interest. This avoids the need for systematic use of embedded models, as is the case with the finite-difference method.

<b>Model</b>	TELEMATAC
<b>Contact</b>	Eric Jones - jej@pol.ac.uk
<b>Link</b>	<a href="http://www.telematacsystem.com/gb/default.html">http://www.telematacsystem.com/gb/default.html</a>
<b>Literature</b>	Jones E. J., and Davies A. M., 2006: Application of a finite element model (TELEMATAC) to computing the wind induced response of the Irish Sea. <i>Continental Shelf Research</i> , <b>26</b> (12-13), 1519-1541.
<b>Code</b>	--
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v5.8 (2007)

#### 3.4.1.12 UK STORM SURGE MODEL

The U.K. Storm Surge Model combines over 1,000 stochastic storm surge events along the U.K. East Coast with associated windfields and their probabilities, allowing a complete view of risk to be assessed. Different tidal states are applied to capture the interaction of the tide with the storm surge. For example, a modest storm that coincides with the highest spring tide of the year may cause a higher water level than a strong storm that occurs on the lowest neap tide of the year.

<b>Model</b>	UK Storm Surge Model
<b>Contact</b>	Kevin Horsburgh - kevinh@pol.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

#### 3.4.1.13 UWB 1DV

The UWB 1DV Sand Transport Model is an intra-wave numerical model which has been developed at Bangor University for sand transport by waves and currents (see Malarkey and Davies, 2005). It can represent both the advectively dominated processes that are typical over a rippled bed as a result of vortex shedding (see Malarkey and Davies, 2004 and Davies and Thorne, 2005) and the more diffusively dominated processes over flat mobile beds.

<b>Model</b>	UWB 1DV
<b>Contact</b>	--
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 4 NERC COLLABORATIVE CENTRES

NERC collaborative centres are funded by contract. They are managed from outside NERC and staff are not usually employed by NERC.

### 4.1 NATIONAL CENTRE FOR ATMOSPHERIC SCIENCE

The National Centre for Atmospheric Science (NCAS) provides a national capability in atmospheric science research. The centre increases knowledge of key environmental issues including: climate change, weather processes and atmospheric composition including air quality. It uses state-of-the-art technologies for observing and modelling the atmosphere and its research is used by policy makers and the wider UK science base. NCAS is not based in one location. It is a collaborative centre made up three science directorates (climate; weather; atmospheric composition) and four services and facilities distributed across many UK universities and related institutions.

#### 4.1.1.1 BLASIUS

Boundary Layer Above Stationary Inhomogeneous Uneven Surfaces (BLASIUS) is a numerical model designed to simulate turbulent flow over hills. As its name suggests, BLASIUS can handle flow over orography such as two- and three-dimensional hills and waves as well as flat surfaces. It can model both laminar and turbulent flow. The boundary conditions at the surface are no-slip for velocity and either constant surface flux, constant surface value or constant available energy for temperature and water vapour. At the top of the domain a zero vertical mass flux is imposed. The boundary conditions for momentum, temperature, water vapour and turbulent kinetic energy can be specified by integer switches in namelists (see documentation for details). Lateral boundary conditions can be either periodic or inflow/outflow. A first order closure is used with the option of carrying turbulent kinetic energy as a prognostic variable. The model can also be used to perform Large Eddy Simulations (LES).

<b>Model</b>	BLASIUS
<b>Contact</b>	Lois Steenman-Clark - L.Steenman-Clark@reading.ac.uk
<b>Link</b>	<a href="http://www.met.reading.ac.uk/~bl_met/UWERN/">http://www.met.reading.ac.uk/~bl_met/UWERN/</a>
<b>Literature</b>	---
<b>Code</b>	FORTRAN 77
<b>Platform</b>	DOS, LINUX, UNIX, VMS
<b>Latest Update</b>	v3.03 (2002)

## 4.1.1.2 CICE

The Los Alamos sea ice model (CICE) is the result of an effort to develop a computationally efficient sea ice component for a fully coupled atmosphere-ice-ocean-land global climate model. It was designed to be compatible with the Parallel Ocean Program (POP), an ocean circulation model developed at Los Alamos National Laboratory for use on massively parallel computers. The current version of the model has been enhanced greatly through collaborations with members of the Community Climate System Model (CCSM) Polar Climate Working Group, based at the National Center for Atmospheric Research (NCAR), and researchers at the U.K. Met Office Hadley Centre.

<b>Model</b>	CICE
<b>Contact</b>	Rosalyn Hatcher - r.s.hatcher@reading.ac.uk
<b>Link</b>	<a href="http://oceans11.lanl.gov/trac/CICE">http://oceans11.lanl.gov/trac/CICE</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN 90
<b>Platform</b>	--
<b>Latest Update</b>	v4.0 (2008)

## 4.1.1.3 GLOMAP

GLOMAP is a global atmospheric aerosol and chemistry model with a comprehensive treatment of aerosol microphysical and chemical processes. The model is being used to study the global lifecycle of aerosol and the impact of aerosol on climate. GLOMAP runs within the TOMCAT Chemical Transport Model and the UKCA aerosol-chemistry-climate model.

<b>Model</b>	GLOMAP
<b>Contact</b>	Ken Carslaw - k.s.carslaw@leeds.ac.uk
<b>Link</b>	<a href="http://researchpages.net/GLOMAP/">http://researchpages.net/GLOMAP/</a>
<b>Literature</b>	Korhonen H., Carslaw K. S., Spracklen D. V., Ridley D. A., and Ström J., 2008: A global model study of processes controlling aerosol size distributions in the Arctic spring and summer. <i>J. Geophys. Res.</i> , 113,
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 4.1.1.4 IGCM

The Reading Intermediate General Circulation Model (IGCM), is a simplified or "intermediate" Global climate model, which is developed by members of the Department of Meteorology at the University of Reading, and by members of the Stratospheric Dynamics and Chemistry Group of the Department of Atmospheric and Oceanic Sciences at McGill University. The IGCM is a fast GCM based on the primitive-equations baroclinic model of Hoskins and Simmons, which has been converted to run on workstations. Several versions have been developed with representations of the physics. IGCM1: Portable version of the original spectral dry baroclinic model formulated in sigma-levels, with an option for Newtonian relaxation and Rayleigh friction, no surface. IGCM2: Includes simplified moist parameterisations, a cheap "radiation scheme" (ie constant tropospheric cooling), a bulk formulation scheme for the boundary layer, fixed surface temperatures and humidity, a uniform vertical diffusion, and can advect tracers. IGCM3x: Intermediate climate model which includes more sophisticated moist / clouds parameterisations, a radiation scheme with various gas absorbers, and a more realistic surface with an orography and land, sea surface schemes.

<b>Model</b>	IGCM
<b>Contact</b>	Mike Blackburn - m.blackburn@reading.ac.uk
<b>Link</b>	<a href="http://www.met.reading.ac.uk/~mike/dyn_models/igcm/">http://www.met.reading.ac.uk/~mike/dyn_models/igcm/</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 4.1.1.5 JULES

JULES is the Joint UK Land Environment Simulator. It is based on MOSES (Met Office Surface Exchange System), the land surface model used in the Unified Model of the UK Met Office (UK Meteorological Service). MOSES was originally designed to represent the land surface in Meteorological and Climate models, but is increasingly used for other purposes: predicting river flows, identifying global wetlands, quantifying water resources.

<b>Model</b>	JULES
<b>Contact</b>	Rosalyn Hatcher - r.s.hatcher@reading.ac.uk
<b>Link</b>	<a href="http://www.jchmr.org/jules">http://www.jchmr.org/jules</a>
<b>Literature</b>	Mercado L. M., Huntingford C., Gash J. H. C., Cox P. M., Jogireddy V., 2007: Improving the representation of radiation interception and photosynthesis for climate model applications. <i>Tellus B</i> , <b>59</b> (3). 553-565.
<b>Code</b>	FORTRAN
<b>Platform</b>	UNIX
<b>Latest Update</b>	v2.1 (2007)

## 4.1.1.6 LEM

The Large Eddy Model (LEM) is also known as the Cloud Resolving Model (CRM). Turbulence is constructed of eddies of varying sizes. In more primitive models this turbulence is completely parameterised by theories relating it to the mean flow. Typically, in the LEM the large eddies are modelled - while only the smaller eddies are parameterised (hence the name, LEM). It's used to simulate a wide range of atmospheric and fluid dynamical problems.

<b>Model</b>	LEM
<b>Contact</b>	--
<b>Link</b>	<a href="http://www.met.reading.ac.uk/~lem/large_models/lem/intro/">http://www.met.reading.ac.uk/~lem/large_models/lem/intro/</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v2.4

## 4.1.1.7 NEMO

Nucleus for European Modelling of the Ocean (NEMO) is an ocean modelling framework which is composed of "engines" nested in an "environment". The "engines" provide numerical solutions of ocean, sea-ice, tracers and biochemistry equations and their related physics. The "environment" consists of the pre- and post-processing tools, the interface to the other components of the Earth System, the user interface, the computer dependent functions and the documentation of the system. NEMO allows several ocean related components of the earth system to work together or separately. It also allows a two-way nesting via the AGRIF software. It is interfaced with the remaining component of the earth system (atmosphere, land surfaces, etc) via the OASIS coupler.

<b>Model</b>	NEMO
<b>Contact</b>	Rosalyn Hatcher - r.s.hatcher@reading.ac.uk
<b>Link</b>	<a href="http://www.nemo-ocean.eu/">http://www.nemo-ocean.eu/</a>
<b>Literature</b>	Lefebvre, W., and Goosse H., 2008 : Analysis of the projected regional sea-ice changes in the Southern Ocean during the twenty-first century, <i>Climate Dynamics</i> , <b>30</b> (1) 59-76,
<b>Code</b>	--
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v3.1 (2008)

## 4.1.1.8 TOMCAT (SLIMCAT)

TOMCAT is a three-dimensional (3D) off-line chemical transport model (CTM). The model uses winds and temperatures from meteorological analyses (e.g. from the UK Met Office or ECMWF) to specify the atmospheric transport and temperatures and calculates the abundances of chemical species in the troposphere and stratosphere. The model has the option of detailed chemical scheme(s) for the stratosphere and troposphere. The model can be used to simulate the past and current atmosphere, and to diagnose the extent of problems such as stratospheric ozone depletion or tropospheric pollution. SLIMCAT is the stratosphere only version of TOMCAT

<b>Model</b>	TOMCAT/SLIMCAT
<b>Contact</b>	Lois Steenman-Clark - L.Steenman-Clark@reading.ac.uk
<b>Link</b>	<a href="http://homepages.see.leeds.ac.uk/~lecmc/slimcat.html">http://homepages.see.leeds.ac.uk/~lecmc/slimcat.html</a>
<b>Literature</b>	Chipperfield M. P., 2006: New version of the TOMCAT/SLIMCAT off-line chemical transport model: Inter-comparison of stratospheric tracer experiments. <i>Q. J. R. Meteorol. Soc.</i> , <b>132</b> , 1179-1203.
<b>Code</b>	FORTRAN 77 and 90
<b>Platform</b>	Windows, UNIX, LINUX
<b>Latest Update</b>	v0.8 (2006)

## 4.1.1.9 UKCA

The UK Chemistry Aerosol Model (UKCA) is a joint programme between NCAS and the UK Met Office programme. The UKCA model has been designed as a component of the Unified Model, and is available from vn6.6 of the UM. UKCA uses the standard tracer transport schemes available in the UM, and uses diagnostics from the atmosphere model which are made available at each timestep. The main components of UKCA are the interface with the UM, stratospheric and tropospheric chemistry schemes, together with aerosols, and components which couple the trace gases and aerosols to the radiation scheme of the UM. The principle task completed in the past year was to bring the entire UKCA model together in version 6.6 of the UM. This report documents the development of the model as coupled to versions of the climate model, but UKCA is now being used in other applications, notably in a prototype air quality model at the Met Office, and is being used together with a nudging scheme to reproduce historical weather using ERA - 40 analyses at Cambridge University.

<b>Model</b>	UKCA
<b>Contact</b>	Graham Mann - gmann@env.leeds.ac.uk
<b>Link</b>	<a href="http://www.ukca.ac.uk/">http://www.ukca.ac.uk/</a>
<b>Literature</b>	Morgenstern O., Braesicke P., O'Connor F. M., Bushell A. C., Johnson C. E., Osprey S. M., and Pyle J. A., 2008: Evaluation of the new UKCA climate-composition model – Part I: The stratosphere, <i>Geosci. Model Dev. Discuss.</i> , 1, 381-432.
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

## 4.1.1.10 UM

The Unified Model (UM) software is designed so that the model can be run in atmosphere-only (global or limited area), ocean-only or in coupled atmosphere-ocean mode. The Unified Model is used by the UK Met Office for operational numerical weather prediction and by the Hadley Centre for Climate Prediction and Research to simulate and predict the Earth's climate.

<b>Model</b>	UM
<b>Contact</b>	Rosalyn Hatcher - r.s.hatcher@reading.ac.uk
<b>Link</b>	<a href="http://ncas-cms.nerc.ac.uk/content/view/67/26/">http://ncas-cms.nerc.ac.uk/content/view/67/26/</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	v6.1 (2009)

## 4.1.1.11 WRF

The Weather Research and Forecasting (WRF) model is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It features multiple dynamical cores, a three dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility. WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometres.

<b>Model</b>	WRF
<b>Contact</b>	Alan Gadian - alan@env.leeds.ac.uk
<b>Link</b>	<a href="http://www.wrf-model.org/index.php">http://www.wrf-model.org/index.php</a>
<b>Literature</b>	Skamarock W. C., 2004: Evaluating Mesoscale NWP Models Using Kinetic Energy Spectra. <i>Mon. Wea., Rev.</i> , <b>132</b> , 3019-3032
<b>Code</b>	FORTRAN, C, C++
<b>Platform</b>	UNIX, LINUX
<b>Latest Update</b>	v3.1 (2009)

## 4.2 NATIONAL OCEANOGRAPHY CENTRE

The National Oceanographic Centre, Southampton (NOCS) is the national focus for oceanography in the UK with a remit to achieve scientific excellence in its own right as one of the world's top five oceanographic research institutions. NOCS delivers a diverse mission, which ranges from managing the national research vessel fleet and other major facilities, to programmes of strategic research for NERC, and academic research and education in ocean and earth sciences in support of the University's mission. NOCS activities also encompass major ocean technology development, long-term observations, managing international science programmes, promoting enterprise and knowledge transfer, providing advice to Government, business and charities, and the engagement between science and society. Moreover, the Centre is also specifically charged with working with the wider science community to provide strategic leadership, coordination and facilitation for the whole of the UK marine and related earth sciences.

### 4.2.1.1 NEMO

The Nucleus for European Modelling of the Ocean (NEMO) is an ocean modelling framework which is composed of "engines" nested in an "environment". The "engines" provide numerical solutions of ocean, sea-ice, tracers and biochemistry equations and their related physics. The "environment" consists of the pre- and post-processing tools, the interface to the other components of the Earth System, the user interface, the computer dependent functions and the documentation of the system. NEMO allows several ocean related components of the earth system to work together or separately. It also allows a two-way nesting via the AGRIF software. It is interfaced with the remaining components of the earth system (atmosphere, land surfaces, etc) via the OASIS coupler. This is the main ocean model in use at NOCS. We have already completed several global hindcasts covering 1958-2001, and are now starting on a global 1/12° integration. The MEDUSA ecosystem model has been embedded within NEMO and tests are underway at 1/4°. We have been using the LIM2 and LIM3 sea-ice models, but are now also starting work with the CICE sea-ice model.

<b>Model</b>	NEMO
<b>Contact</b>	Adrian New - a.new@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.nemo-ocean.eu/">http://www.nemo-ocean.eu/</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN
<b>Platform</b>	HeCTOR National HPC facility; SGI-Altix cluster at NOCS.
<b>Latest Update</b>	v3.2 (2009)

### 4.2.1.2 MEDUSA

The Model of Ecosystem Dynamics, nutrient Utilisation and SequestrAtion (MEDUSA) is a size-based plankton ecosystem model of the biogeochemical cycles of nitrogen, silicon and iron that has been developed to explore *Oceans 2025* goals. Work with MEDUSA is focused on high-resolution, multi-decadal variability (hindcasts) of biogeochemical cycles at the global scale. Current activity is directed at preliminary testing of short duration simulations in full 3D NEMO (1° and 1/4°), and the initiation of a "forced" hindcast (1958 to 2001). This simulation restores deep nutrient concentrations to observational fields, and analysis of its results will diagnose MEDUSA deficiencies.

<b>Model</b>	MEDUSA
<b>Contact</b>	Tom Anderson - tra@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.nemo-ocean.eu/content/download/7563/41014/file/Andrew_Yool.ppt">http://www.nemo-ocean.eu/content/download/7563/41014/file/Andrew_Yool.ppt</a>
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

#### 4.2.1.3 CHIME

The Coupled Hadley-Isopycnic Model Experiment (CHIME) comprises a new coupled climate model, developed at the National Oceanography Centre, Southampton. It consists of the atmospheric model used in the Hadley Centre's HadCM3 climate model, coupled to a hybrid coordinate ocean model (HYCOM) via the OASIS coupler. The ocean model grid is identical over most of the globe to that used in HadCM3, allowing the effect of the different vertical representation of the ocean to be easily assessed. In particular, HyCOM should provide a better representation of the ocean's individual water masses than is achieved by HadCM3. A further innovative feature of CHIME's ocean component is its use of a bipolar grid over the Arctic. This avoids the problem of convergence of meridians toward the North Pole by replacing the latitude-longitude grid in HadMC3 north of a given latitude circle with a bipolar grid. This matches the spherical grid perfectly at this latitude, but its two poles may be placed harmlessly in large land masses.

<b>Model</b>	CHIME
<b>Contact</b>	Alex Megann – apm@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.noc.soton.ac.uk/JRD/LSM/CHIME/">http://www.noc.soton.ac.uk/JRD/LSM/CHIME/</a>
<b>Literature</b>	--
<b>Code</b>	Fortran 90
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	v2.1.34

#### 4.2.1.4 C-GOLDSTEIN

C-GOLDSTEIN is a frictional geostrophic ocean model coupled to a simplified energy-moisture balance atmospheric model and a thermodynamic sea ice model, the first step towards a very fast Earth System Model to simulate climate variability on millennial timescales. C-GOLDSTEIN underpins the NERC e-Science project GENIE (Grid ENabled Integrated Earth system modelling).

<b>Model</b>	C-GOLDSTEIN
<b>Contact</b>	Bob Marsh - rma@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.soc.soton.ac.uk/JRD/LSM/CGOLD/">http://www.soc.soton.ac.uk/JRD/LSM/CGOLD/</a>
<b>Literature</b>	Marsh R., Edwards N. R., and Shepherd J. G., 2002: Development of a fast climate model (C-GOLDSTEIN) for Earth System Science. <i>Southampton Oceanography Centre Internal Document</i> , <b>83</b> , 50.
<b>Code</b>	FORTRAN
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	v2 (2003)

#### 4.2.1.5 FORTE

FORTE (Fast Ocean Rapid Troposphere Experiment) is a coarse resolution ocean-atmosphere coupled general circulation model capable of integrations over timescales ranging from days to thousands of years. It is also capable of a high degree of flexibility - the model has been designed with the intention of performing experiments using highly idealised configurations, so it can accept new continental geometry, land surface orography and ocean bottom topography easily; the resolution of the ocean (and to a lesser extent, the atmosphere) is also configurable. Its principal components are ocean and atmosphere General Circulation Models (GCMs) originally designed for solo operation.

<b>Model</b>	FORTE
<b>Contact</b>	Bablu Sinha - B.Sinha@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.noc.soton.ac.uk/JRD/LSM/FORTE/">http://www.noc.soton.ac.uk/JRD/LSM/FORTE/</a>
<b>Literature</b>	Sinha B., and Smith R. S., 2002: Development of a fast Coupled General Circulation Model (FORTE) for climate studies, implemented using the OASIS coupler. <i>Southampton Oceanography Centre Internal Document</i> , <b>81</b> , 67.
<b>Code</b>	--
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

#### 4.2.1.6 LIM

Within the Louvain-la-Neuve Sea Ice Model (LIM) sensible heat storage and vertical heat conduction within snow and ice are determined by three layers (one layer for snow and two layers for ice). The effect of the subgrid-scale snow and ice thickness distributions is accounted for through an effective thermal conductivity, which is computed by assuming that the snow and ice thicknesses are uniformly distributed between zero and twice their mean value over the ice-covered portion of the grid cell. The storage of latent heat inside the ice resulting from the trapping of shortwave radiation by brine pockets is taken into account. An albedo formulation takes into consideration the state of the surface (frozen or melting) and the thickness of the snow and ice covers. The model also allows for the presence of leads within the ice pack. Vertical and lateral growth/decay rates of the ice are obtained from prognostic energy budgets at both the bottom and surface boundaries of the snow-ice cover and in leads.

<b>Model</b>	LIM2 and LIM3
<b>Contact</b>	Yevgney Aksenov - yka@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.astr.ucl.ac.be/index.php?page=vancop%23LIM3">http://www.astr.ucl.ac.be/index.php?page=vancop%23LIM3</a>
<b>Literature</b>	Danilov S., Schröter J., Böning C., Sidorenko D., and Rollenhagen K., 2008: Ocean circulation and sea ice distribution in a finite element global sea ice–ocean model. <i>Ocean Modelling</i> , <b>3-4</b> , 114-129.
<b>Code</b>	FORTRAN 90
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	v3 (2008)

#### 4.2.1.7 CICE

The Los Alamos sea ice model (CICE) is the result of an effort to develop a computationally efficient sea ice component for a fully coupled atmosphere-ice-ocean-land global climate model. It was designed to be compatible with the Parallel Ocean Program (POP), an ocean circulation model developed at Los Alamos National Laboratory for use on massively parallel computers. The current version of the model has been enhanced greatly through collaborations with members of the Community Climate System Model (CCSM) Polar Climate Working Group, based at the National Center for Atmospheric Research (NCAR), and researchers at the U.K. Met Office Hadley Centre.

<b>Model</b>	CICE
<b>Contact</b>	Yevgney Aksenov - yka@noc.soton.ac.uk
<b>Link</b>	<a href="http://oceans11.lanl.gov/trac/CICE">http://oceans11.lanl.gov/trac/CICE</a>
<b>Literature</b>	--
<b>Code</b>	FORTRAN 90
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

#### 4.2.1.8 MICOM

The Miami Isopycnic-Coordinate Ocean Model (MICOM) is used to investigate the circulation and processes in the World Ocean. This work is part of that undertaken by the Large-Scale modelling team in the James Rennell Division for Ocean Circulation and Climate. This work started in 1990, initially implementing a model of the North Atlantic (using monthly climatological forcing and realistic bathymetry and initial conditions) at a horizontal resolution of about 1 degree, in the AIM (Atlantic Isopycnic Model) project. The model was spun-up for several decades and used to study the ventilation of the subtropical gyre, patterns of tracer distributions, inter-decadal variability of the upper ocean water masses, and water mass formation rates. The model was also compared with a Bryan-Cox level model set up by the Hadley Centre for Climate Prediction and Research (part of the UK Met. Office) to be as similar as possible, and major differences were noted to result from the way in which the two models handled the overflows of the deep water masses from the Greenland-Iceland-Norwegian Seas.

<b>Model</b>	MICOM
<b>Contact</b>	Alex Megann - apm@noc.soton.ac.uk
<b>Link</b>	Alex – give correct url from Naval Research Lab at Stennis Space Centre in the US or wherever – the original link here was to knmi.
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

#### 4.2.1.9 HYCOM

This is the successor to MICOM. It is a Hybrid coordinate ocean model in which the ocean interior comprises a set of constant density layers (isopycnals). These transition to constant-depth z-levels near the surface. HyCOM forms the ocean component of the CHIME coupled climate model.

<b>Model</b>	HyCOM
<b>Contact</b>	Alex Megann - apm@noc.soton.ac.uk
<b>Link</b>	Alex – give correct url from Naval Research Lab at Stennis Space Centre in the US
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

#### 4.2.1.10 OCCAM

The OCCAM model is based on the Bryan-Cox-Semtner ocean general circulation model. Bryan developed the initial version of the model but Semtner and Cox made important contributions which helped its rapid acceptance by the oceanographic community. The model is based on the ocean primitive equations; its main difference from other ocean models is the use of an Arakawa-B grid in the horizontal and level surfaces in the vertical. Work at NOCS has developed OCCAM as a particularly efficient code to run on massively parallel High Performance Computing platforms.

<b>Model</b>	OCCAM
<b>Contact</b>	Andrew Coward - a.coward@noc.soton.ac.uk
<b>Link</b>	<a href="http://www.noc.soton.ac.uk/omf/research/occam/">http://www.noc.soton.ac.uk/omf/research/occam/</a>
<b>Literature</b>	Saunders P. M., Coward A. C., and de Cuevas B. A., 1999: Circulation of the Pacific Ocean seen in a global ocean model (OCCAM). <i>J. Geophys. Res.</i> , <b>104</b> (C8), 18281-18299.
<b>Code</b>	--
<b>Platform</b>	HeCTOR National HPC platform
<b>Latest Update</b>	--

## 4.2.1.11 MITGCM

The MITGCM is a non-hydrostatic ocean general circulation model which we are using to study the generation and propagation of internal waves in the ocean.

<b>Model</b>	MITGCM
<b>Contact</b>	George Nurser - agn@noc.soton.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	--
<b>Platform</b>	SGI-Altix cluster at NOCS
<b>Latest Update</b>	--

## 4.2.1.12 ICOM

ICOM is an unstructured ocean circulation which is now in development and will offer capability of adaptive gridding. That is, the ocean model grid adapts to put extra resolution where the gradients in the flow are sharpest. The model development is led by Imperial College in London, but NOCS are involved to assist in its development.

<b>Model</b>	ICOM
<b>Contact</b>	Adrian New - anw@noc.soton.ac.uk
<b>Link</b>	--
<b>Literature</b>	---
<b>Code</b>	--
<b>Platform</b>	--
<b>Latest Update</b>	--

### 4.3 PLYMOUTH MARINE LABORATORY

Research programmes Plymouth Marine Laboratory (PML) are focused on solving the complexities within marine ecosystems and developing relevant and integrated approaches for delivering a sustainable basis to marine ecosystem management and understanding the role of the oceans in the Earth System. We contribute to timely and highly relevant research for both UK and international societal needs. Our research tackles areas of major concern to humankind such as global change, pollution and sustainability. Playing an integral part in the UK's strategic marine science and technology capability for over 30 years, they advise Government, the European Union and international regulating bodies on strategic issues ranging from the 'ecosystem approach' to global change issues such as ocean acidification.

#### 4.3.1.1 ERSEM

The European Regional Seas Ecosystem Model (ERSEM) was conceived as a generic model, when coupled to a qualitatively correct physical model. It is designed to be capable of correctly simulating the spatial pattern of ecological fluxes throughout the seasonal cycle and across eutrophic to oligotrophic gradients. There are perhaps three reasons that allow ERSEM this flexibility. Firstly it includes detailed representations of the benthic system, which are vital for the correct treatment of shelf seas. Secondly it decouples carbon and nutrient dynamics which gives a far better approximation to how nutrient limitation acts on cells. Thirdly it can simulate both the "classical" large cell production / grazing dynamics and the small cell microbial loop, thereby representing the continuum of trophic pathways evident in marine systems. Recent modifications to ERSEM include the inclusion of carbon chemistry, Fe limitation, the response of organisms to ocean acidification and DMS production.

<b>Model</b>	ERSEM
<b>Contact</b>	Icarus Allen - <a href="mailto:jia@pml.ac.uk">jia@pml.ac.uk</a>
<b>Link</b>	<a href="http://web.pml.ac.uk/ecomodels/ersem.htm">http://web.pml.ac.uk/ecomodels/ersem.htm</a>
<b>Literature</b>	Blackford et al J Mar Sys 2004
<b>Code</b>	FORTRAN
<b>Platform</b>	LINUX, HECTOR
<b>Latest Update</b>	2009

#### 4.3.1.2 GOTM-ERSEM

General Ocean Turbulence Model (GOTM) is a one-dimensional water column model for the most important hydrodynamic and thermodynamic processes related to vertical mixing in natural waters. In addition, it has been designed such that it can easily be coupled to 3-D circulation models, and used as a module for the computation of vertical turbulent mixing. The core of the model computes solutions for the one-dimensional versions of the transport equations of momentum, salt and heat. The key component in solving these equations is the model for the turbulent fluxes of these quantities. The strength of GOTM is the vast number of well-tested turbulence models that have been implemented in the code. These models span the range from simple prescribed expressions for the turbulent diffusivities up to complex Reynolds-stress models with several differential transport equations to solve. Even though, evidently, not all turbulence models published in oceanography could be implemented, at least one member of every relevant model family can be found in GOTM: empirical models, energy models, two-equation models, Explicit Algebraic Stress Models (EASM), and K-profile parameterisations (KPP). ERSEM has been coupled to ERSEM and provides a globally re-locatable water column modelling system for process studies.

<b>Model</b>	GOTM
<b>Contact</b>	Jerry Blackford - jcb@pml.ac.uk
<b>Link</b>	<a href="http://www.gotm.net/pages/documentation/manual/pdf/a4.pdf">http://www.gotm.net/pages/documentation/manual/pdf/a4.pdf</a>
<b>Literature</b>	Allen et al J Sea Res 2004.
<b>Code</b>	FORTRAN
<b>Platform</b>	Windows, LINUX
<b>Latest Update</b>	v4.0 (2007)

#### 4.3.1.3 MRCS/ATLANTIC MARGIN

The MRCS (Medium-Resolution Continental Shelf) model is a coupled hydrodynamic-ecosystem model, nested within the Atlantic Margin Model. The hydrodynamics are supplied by the Proudman Oceanographic Laboratory Coastal Ocean Modelling System (POLCOMS) and the ecosystem component is supplied by the European Regional Seas Ecosystem Model (ERSEM). An operational version is run by the met office.

<b>Model</b>	MRCS/AMM
<b>Contact</b>	Momme Butenschon - momm@pml.ac.uk
<b>Link</b>	<a href="http://www.ncof.co.uk/Coastal-Seas-Model-Description.html">http://www.ncof.co.uk/Coastal-Seas-Model-Description.html</a>
<b>Literature</b>	Allen et al 2001 Sarsia
<b>Code</b>	FORTRAM
<b>Platform</b>	HECTOR, linux cluster
<b>Latest Update</b>	2009

## 4.3.1.4 GCOMS

GCOMS (Global and Coastal Observation Model). The aim of the Testbed project is to establish a numerical model system providing a robust three dimensional physical environment within which ecosystem and zooplankton models of differing structure and complexity will be compared and assessed. The work is central to the main themes of NERC's Marine Productivity thematic: "To construct and validate spatially explicit models of zooplankton and their food and predators, capable of resolving short term changes in population structure" and "To identify the dominant spatial and temporal scales of physical parameters and zooplankton population dynamics, by observation, modelling and retrospective analysis".

<b>Model</b>	GCOMS / QUEST FISH
<b>Contact</b>	Rob Holmes – robe1b@pml.ac.uk
<b>Link</b>	--
<b>Literature</b>	Holt et al 2009 Proc R Soc A Barange et al 2009
<b>Code</b>	FORTAN
<b>Platform</b>	HECTOR
<b>Latest Update</b>	--

## 4.3.1.5 WCH

Based on POLCOMS-ERSEM the Western English Channel (WCH) model domain is set up as a subset of the larger Medium Resolution Continental Shelf domain (MRCS) of the north-west European Continental Shelf, at a resolution of approximately 7km. A 1nm model is also been set-up as a pre-operational model.

In both cases the domain has been forced with boundary conditions extracted from MRCS simulations run at POL and the UK Met Office for the years 2003-2009 and currently runs in a pre-operational mode, with weekly hindcast data being provided by the UK Met Office. Surface forcing is provided by the PML Met' Station. The domain is being used as a test-bed for Ensemble Kalman filter data assimilation of satellite ocean colour data.

<b>Model</b>	WCH
<b>Contact</b>	Ricardo Torres - rito@pml.ac.uk
<b>Link</b>	--
<b>Literature</b>	Lewis et al J mar Sys 2009
<b>Code</b>	FORTTRAN
<b>Platform</b>	PML cluster
<b>Latest Update</b>	2009

## 4.3.1.6 NEMO\_ERSEM

ERSEM is being coupled to a 1 degree global ocean NEMO model supplied by NOCS.

<b>Model</b>	NEMO-ERSEM
<b>Contact</b>	Momme Butenschon - momm@pml.ac.uk
<b>Link</b>	--
<b>Literature</b>	--
<b>Code</b>	FORTRAN
<b>Platform</b>	PML cluster
<b>Latest Update</b>	--

## 4.4 SCOTTISH ASSOCIATION FOR MARINE SCIENCE

The Scottish Association for Marine Science (SAMS) is one of the oldest oceanographic organisations in the world. It operates the Dunstaffnage Marine Laboratory - three miles north of Oban in Scotland - and hosts the National Facility for Scientific Diving and the Culture Collection of Algae and Protozoa. It is an internationally renowned marine centre that focuses much of its activities on multidisciplinary research questions from Scottish coastal waters to the Arctic Ocean. Its core science programme investigates past and present changes in northern seas. Much of the research is inter-disciplinary, for example their work on climate change or marine renewable energy. It involves close collaboration between research groups within our four departments; ecology; biogeochemistry and Earth Sciences; microbial and molecular; and physics, sea ice and technology.

### 4.4.1.1 DEPOMOD

A particle tracking model used for predicting flux of particulate waste material (with re-suspension) and associated benthic impact of fish farms. Simulated particles sink and are displaced by currents and random-walk eddy dispersion. Shear in the water column can be represented by layers in the model. Re-suspension is a function of near-bed currents. Benthic community impact is predicted by an empirical relationship between depositional flux and the ITI. Sediment content of a particulate component, such as a medicine, can also be predicted.

<b>Model</b>	DEPOMOD
<b>Contact</b>	Chris Cromey - chjc@sams.ac.uk
<b>Link</b>	<a href="http://www.sepa.org.uk/water/aquaculture/marine_aquaculture/fish_farm_manual.aspx">http://www.sepa.org.uk/water/aquaculture/marine_aquaculture/fish_farm_manual.aspx</a> (Annex H)
<b>Literature</b>	Cromey C. J., Nickell T. D., Black K. D., Provost P. G., and Griffiths C. R., 2002: Validation of a fish farm waste re-suspension model by use of a particulate tracer discharged from a point source in a coastal environment. <i>Estuaries</i> , <b>25</b> , 916-929.
<b>Code</b>	Borland Delphi 7
<b>Platform</b>	Windows
<b>Latest Update</b>	v3.0 (2005)

## 4.5 UK ENERGY RESEARCH CENTRE

The mission of the UK Energy Research Centre (UKERC) is to be the UK's pre-eminent centre of research on sustainable energy systems. To achieve this, the centre is establishing a comprehensive database of energy research, development and demonstration competences in the UK. The centre will also act as the portal for the UK energy research community to and from both UK stakeholders and the international energy research community.

### 4.5.1.1 MARKAL

MARKAL (acronym for MARKet ALlocation) is a widely applied bottom-up, dynamic, linear programming (LP) optimisation model. It supported by the International Energy Agency (IEA) via the Energy Technology and Systems Analysis Program (ETSAP). The IEA is currently developing a multi-region version of the model, precisely to consider the kinds of issues – technology choices under a CO<sub>2</sub> constraint – that we have examined for the UK. Technologies are assumed to be developed globally and to benefit from advances in design, engineering and production stemming from such broad involvement, although the implications of more limited innovation have been explored. It is being used by around 100 active teams in over 30 countries, and has a long track record of policy and academic research. MARKAL portrays the entire energy system from imports and domestic production of fuel resources, through fuel processing and supply, explicit representation of infrastructures, conversion to secondary energy carriers (including electricity, heat and hydrogen), end-use technologies and energy service demands in the industrial, commercial, residential, transport and agricultural sectors.

<b>Model</b>	MARKAL
<b>Contact</b>	Nick Hughes - nick.hughes@kcl.ac.uk
<b>Link</b>	<a href="http://www.ukerc.ac.uk/ResearchProgrammes/EnergySystemsandModelling/ESMMARKALDocs08.aspx">http://www.ukerc.ac.uk/ResearchProgrammes/EnergySystemsandModelling/ESMMARKALDocs08.aspx</a>
<b>Literature</b>	Ekins P., Kannan R., and Strachan N., 2007: The Structure and Use of the UK MARKAL Model. SEEC International handbook on the economics of energy, University of Surrey, UK.
<b>Code</b>	DOS, OMNI, FORTRAN
<b>Platform</b>	Windows
<b>Latest Update</b>	--

## 4.5.1.2 MDM-E3

The Cambridge Multisectoral Dynamic Model of the UK economy (MDM-E3), is maintained and developed by CE as a framework for generating forecasts and alternative scenarios, analysing changes in economic structure and assessing energy-environment-economy (E3) issues and other policies. MDM-E3 provides a one-model approach in which the detailed industry and regional analysis is consistent with the macroeconomic analysis: in MDM-E3, the key indicators are modelled separately for each industry sector, and for each region, yielding the results for the UK as a whole. MDM-E3 is one of a family of models which share the same framework, general design, methodology, and supporting software; the scope of the E3ME model is European; that of E3MG is global.

To analyse structure, the E3 models disaggregate industries, commodities, and household and government expenditures, as well as foreign trade and investment, and the models incorporate an input-output framework to identify the inter-relationships between industry sectors. The E3 models combine the features of an annual short- and medium-term sectoral model estimated by formal econometric methods with the detail and structure of input-output models, providing analysis of the movement of the long-term outcomes for key E3 indicators in response to economic developments and policy changes. The models are essentially dynamic simulation models estimated by econometric methods.

<b>Model</b>	MDM-E3
<b>Contact</b>	Philip Summerton - ps@camecon.com
<b>Link</b>	<a href="http://www.camecon.com/suite_economic_models/mdme3.htm">http://www.camecon.com/suite_economic_models/mdme3.htm</a>
<b>Literature</b>	Barker T., Ekins P., and Foxon T., 2007: The macro-economic rebound effect and the UK economy. <i>Energy Policy</i> , <b>35</b> (10), 4935-4946.
<b>Code</b>	Oxmetrics 4, FORTRAN, IDIOM
<b>Platform</b>	--
<b>Latest Update</b>	(2003)

## 5 Summary

This report has detailed a model code inventory for the NERC centres, surveys, and time limited collaborative centres. Its aim was to determine the range of model codes used by NERC institutions to enable the DAEM project to scope out the proposed EMP. What is apparent is that there are a large number of model codes used within NERC both bespoke and developed by organisations outside NERC. It is hoped that the inventory will be kept up to date so that environmental researchers in the UK and the rest of the world can use it as a resource.

## References

British Geological Survey, 2009. British Geological Survey strategy 2009-2014. Applied geoscience for a changing earth. British Geological Survey, Nottingham, UK.

Giles, J.R.A., Hughes A.G., Kessler, H., Baker, G., Sen M., Bell P., Peach D. and Moore R.V., 2010. Scoping study for the DAEM project, Open File report OR/10/001. British Geological Survey, Nottingham, UK.