NRA

National Rivers Authority
Anglian Region

TECHNICAL NOTE

USER NOTES FOR THE DEBEN GROUNDWATER MODELLING PACKAGE

Introduction

The full Deben Catchment Modelling Package comprises of several modules, presented as executable files. In brief, use of the package involves linked stages which are outlined in detail below. A computation of the recharge model for the catchment is run and the data output file from this is used as the recharge input file for an adapted version of the USGS groundwater flow model, MODFLOW. The output files from the MODFLOW program are processed using several, specifically written, utility programs.

The various programs are now presented in more detail. As agreed with NRA the following notes assume an understanding of FORTRAN coding, surface water and groundwater modelling techniques and the USGS groundwater model, MODFLOW. The details explained below relate to the application of these to the Deben project work alone.

Recharge Program

The recharge program has been written to define recharge and run-off components specific to the Deben catchment, as stated in the Deben Groundwater Investigation Phase II Report (Hydrotechnica, 1993).

The recharge program, as currently structured, is too big to run on a standard PC DOS configuration, ie 640Kb memory. A computer with additional memory and a FORTRAN compiler which can utilise this are currently required.

The program opens the following input data files:

LANDUSE	-	The proportion of each cell attributed to each landuse type
RSTNMAP3	-	Rainguage identifiers attaching rain gauges to model cells
PEVAP	-	Mean daily potential evaporation data (mm)
RAINFALL	-	Daily rainfall data (mm)
RTCONST	-	Monthly root constants for annual cycle (mm)
FRACTVAR	-	The area in each model cell subject to variable recharge (m^2)
RRCELLS.DAT	-	Links boulder clay runoff cells with runoff-recharge cells

and outputs the files, including:

SSRECHxxx.CSV	-	Steady State Recharge model array for input to MODFLOW

and the water budgeting information:

DRRECHxxx.CSV	-	Direct Recharge array (steady state)
CRRECHxxx.CSV	-	Constant Rate Recharge array (steady state)
RORECHxxx.CSV	-	Runoff-Recharge array (steady state)
NRRECHxxx.CSV	-	Zero Recharge cells identified in code
SSSRUNxxx.CSV	-	Surface Runoff array (steady state)

The character spaces ‘xxx’ in the above file names are available to define the model run no. under consideration. For example the baseline model reported in the Deben Phase II report uses model run no. 29a, therefore the relevant file names are SSRECH29A.CSV, DRRECH29A.CSV, etc, etc.

Model parameters and values as currently set in the recharge program are as follows:

RRMax	Runoff recharge limit to any one cell in any one day (2.5 mm)
NMR1	No. of months indirect recharge retarded (0)
NMR2	No. of months interflow recharge retarded (0)
NMR3	No. of months intercell runoff retarded (0)
RechCon	Constant recharge term (0.05 mm/d = 18 mm/a)
PEFix	Catchment correction to larger scale MORECS square data (1.05)
FIntFlow	% of potential recharge to become interflow (10%)
FIndRech	% of runoff over variable recharge areas to become recharge (5%)
RunRech	% of runoff over constant recharge areas to become recharge (10%)

Note that the model file names and parameters are 'hard wired' into the code. To change any of these it is therefore necessary to edit and re-compile the source code. Relevant parts of the model code can be found using the search facility in any standard text editor.

Groundwater Flow Model

The USGS program MODFLOW has been adapted for the Deben Catchment Model and includes modules specific to the problems encountered. Principal changes from the conventional MODFLOW program include use of a PCG solver and the inclusion of a cell re-wetting subroutine that allows cells that dry out (i.e. the groundwater head falls below the aquifer base) during the iteration procedure to re-wet for the computation in the next iteration. A problem with the restriction of the compiler to DOS conventional memory has made it necessary to remove several unused MODFLOW modules including the SIP and SOR numerical solvers, the drain module and the evapotranspiration module. The large X-array in the program which acts as a general address for passing data between subroutines in the MODFLOW program is set to a dimension of ~~48000~~ 60 000 and this limits the size of the model run to the current Deben catchment.

To reduce the disk space taken by the input files required for all the calibration and scenario modelling runs undertaken, common input files were used for several model runs. A file name structure was developed to keep track of which input files were used for each modelling run. The data file name is dependant on which run the file was first developed for and the input unit that the file refers to. The file name structure is set out as:

debXXXaa.ext (e.g. deb52c10.dat, deb52c.hed & deb52c.uop)

where:

ext specifies the type of file	hed, def for formatted output files uop for unformatted output files dat for data input files
XXX	is the run number that the file was first created in
aa	is the unit number of the file (e.g. 10 for the basic file).

To adapt a previous modelling run for a new scenario the relevant unit, input files need to be modified for the new scenario and saved under the current run number. The run input file (debXXX.in) is then adapted for the new run and all output files corrected to the current run number.

MODDEB is then run with the command:

MODDEB < debXXX.in > out.dat

The program reads the files stated in debXXX.in and outputs the model iteration count to a file out.dat. The iteration count is the number of times that the model must compute a solution for the head calculation to converge to criteria set in the PCG data file. It is, of course, necessary either to have MODDEB.EXE in the same directory as the input files specified in debXXX.in or to have specified the execution path.

The input and output files to MODDEB are allocated to unit numbers within the program which are used to specify the relevant file names. The unit numbers refer to:

Unit:	No:	Description:
BAS	10	Basic Control File
BCF	22	Block Centred Flow Package Input
WEL	23	Well Package Input
RIV	25	River Package Input
GHB	28	General Head Boundary Package Input
RCH	29	Recharge Package Input
OC	33	Output Control File
PCG	34	PCG Package Input
---	69	Dummy file

The program then produces several output files in formatted ASCII and unformatted binary. These are:

File:	Description:
debXXX.hed	Formatted output file of the groundwater head at each node for both layers.
debXXX.def	Formatted output file of the model definition.
debXXX40.uop	Unformatted output file of the cell by cell flow terms.
debXXX45.uop	Unformatted output file of the baseflow component at the river nodes.
debXXX48.uop	Unformatted output file of the flow components along the general head boundary nodes.
debXXX20.uop	Unformatted output file of the groundwater heads at each node.

Utility Programs

Several utility programs have been written to process the unformatted (binary) output files into results sheets for the model run and produce a file format suitable for import into the SURFER contouring package. All the utilities assume new output files, therefore for secondary runs of the same run name the original output files must be removed. The utilities presented are found as executable files on the floppy disc provided and are detailed below:

1. Root Mean Square *

The root mean square analysis, described in our Phase II Report, is available using the program RMS2.EXE. This compares estimated steady state groundwater levels, from observations at specific boreholes, with the model generated groundwater heads for the cell

* See additional note also

associated with each borehole. The program is run by typing RMS2 and then pressing the carriage return. The user is then prompted for relevant information and the results are output as tables for each layer to a file debXXX.rms where XXX is the model run no. The RMS program has been developed for steady state usage only.

2. Baseflow Hydrographs *

The total baseflow for four river reaches, Naunton Hall (NH), Playford (PL), Waldringfield (WL) and Woodbridge (WD), are calculated for each time step and output to a file in CSV format. The output file names are derived from a combination of the abbreviated name of the river reach, the run name and the '.riv' extension, eg NHDEB029A.RIV. The program is run by using BASEQT.EXE which prompts the user for the required information.

3. Groundwater Level Hydrographs *

The program HEADT.EXE extracts groundwater head time series data from the MODFLOW unformatted (binary) results file and outputs the data in CSV format. The results file name is specified by the run name and a 'tpl' extension. Up to 10 cell locations can be specified. The user is prompted for details of this information in the program introduction.

4. Accreted Baseflows and General Head Boundary Flow Calculation

The net baseflow and general head boundary flows are, for steady state simulations, summed along each river reach and the subsequent loss or gain to the reach calculated. The program is run using BASEQ3.EXE and the input file debXXX45.uop, which may be output from MODLFOW. The results are output to a file debXXX.riv specified for each reach within each layer.

5. Surfer Input File *

A file of head data for import into the SURFER contouring package is produced by using SMAKE100D.EXE. The program is run using an input file CMAKE.PI which specifies the input variables. CMAKE.PI should contain the following parameters:

Deben Steady State — Title
MODEL RUN } — Title
DEBXXX — Basic Input Package File used in the run
debXXX10.dat — Block Centred Flow Package Input used in the run
debXXX22.dat — Unformatted output head File
debXXX20.uop — Name of output file, run no. XXX, layer i
debXXXi.dat — Stress period and time step required
1,1 — Layer for the output file
i — Groundwater heads to be output
h

The program is run using the command:

SMAKE100~~D.EXE < CMAKE.PI~~ just type SMAKE100

and will need to be run twice - once for each layer. The output file has the file name stated in MAKE.PI and should be changed for each layer. The data contained are the X and Y coordinates for the cell node location and the groundwater head (Z coordinate). To contour the output groundwater head data import the files created into the GRID module of the SURFER package - for more details on SURFER refer to the user manual.

* See additional notes also

ADDITIONAL NOTES FOR USE WITH HYDROTECHNICA'S USER INSTRUCTIONS

Utility 1 — **Program RMS2.EXE**

Ensure obsgw1.csv & obsgw2.csv are present in the current working directory.

Type RMS2 to start the programs execution.

Input model run name : requires a file name produced by the program MODDEB.EXE

DEB???20.UOP

e.g. DEB59C20.UOP

output in this case would be sent to a file called DEB59C.RMS

Utility 2 — **Program BASEQT.EXE**

Requires the files GHBCAT.DAT & RIVCAT.DAT to be present in the current working directory.

Type BASEQT to start the program execution.

Input model run name : requires an unformatted output file produced by MODDEB.EXE

e.g. DEB???40.UOP

Output to RIV files.

Utility 3 — **HEADT**

Input File : e.g. DEB59C No extension required

Utilities 2 & 3 — **(base flow and gw level hydrographs)**

Will only produce single final values for steady state output.

Utility 5 — **Program SMAKE100.EXE**

Ensure that the files stated within the file CMAKE.P1 are present in the current directory.

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22 April 1994

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Dear Pauline

DEBEN MODEL HANDOVER

Herewith is the Deben Modelling Package and related utilities as promised.

As we discussed, within our estimated budget we have not been able to get the recharge model working on a standard IMB PC compatible due to the memory limitations of this environment. I confirm therefore that the recharge model source code supplied herewith is that which we have used on our HP mini-computer for the Deben Contract. As discussed, you may well be able to get this source code working on your VAX computer with relatively little effort and we therefore await your comments in this respect.

The enclosed software is, to the best of our knowledge, working correctly within the context for which it is intended. However, it is in the nature of modelling work that users may wish to test ideas that extend beyond the scope or range of inputs which the programs were originally intended. In providing this software Entec Hydrotechnica undertakes to correct any programs which may prove to give incorrect results - so long as their use is within the context for which the programs were originally written.

The programs should always be used by experienced hydrogeologists and model results checked against expectations and/or physical plausibility.

Entec Hydrotechnica accepts no liability of any kind should the programs supplied be modified other than by Entec Hydrotechnica and its agents.

Entec Hydrotechnica may charge for costs incurred as a result of inappropriate use of, or modification to, the software.

I trust that the above is clear. However, should you require any clarification or further information, please do not hesitate to contact me.

Yours sincerely

D Russell

Duncan Russell
Senior Hydrogeologist

Enc. 12148C017
12148C019
Floppy Discs

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Dear Stuart

DEBEN MODEL UTILITY FILES

The enclosed disk has another copy of all the utility executables together with copies of:

ghbcat.dat
rivcat.dat

which define the river and general head boundary nodes and are used with the utility Baseqt. The program rms2.exe uses the data files:

obsgw1.csv
obsgw2.csv

to compute an RMS comparison of the model heads to the observed field heads.

The surfer utility SMake100D.exe uses an input file CMake.Pi to define the X, Y and Z co-ordinates.

If you have any other questions please do not hesitate to contact me.

Yours sincerely

RGChurch

Richard Church
Hydrogeologist

Enc: Disk