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TSPROC – A general time-series processor to assist in model calibration and result summarization

By S. Westenbroek, J. Doherty, and J. Walker

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# Preface

Performance of this computer program has been tested and verified for many test cases; however, future applications of the program could reveal errors that were not detected in the test cases. Users are requested to notify the U.S. Geological Survey (USGS) if errors are found in the documentation report or in the computer program.

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The TSPROC code and other model-related programs are available for download­ing from the USGS at the following world wide web address: *http://water.usgs.gov/software/ground\_water.html*.

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Conversion Factors

Inch/Pound to SI

|  |  |  |
| --- | --- | --- |
| Multiply | By | To obtain |
| Length | | |
| inch (in.) | 2.54 | centimeter (cm) |
| foot (ft) | 0.3048 | meter (m) |
| mile (mi) | 1.609 | kilometer (km) |
| Area | | |
| acre | 0.4047 | hectare (ha) |
| acre | 0.004047 | square kilometer (km2) |
| square mile (mi2) | 2.590 | square kilometer (km2) |
| Volume | | |
| cubic foot (ft3) | 0.02832 | cubic meter (m3) |

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

°F=(1.8×°C)+32

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C=(°F-32)/1.8

SI to Inch/Pound

|  |  |  |
| --- | --- | --- |
| Multiply | By | To obtain |
| Length | | |
| centimeter (cm) | 0.3937 | inch (in.) |
| meter (m) | 3.281 | foot (ft) |
| kilometer (km) | 0.6214 | mile (mi) |
| Area | | |
| square meter (m2) | 0.0002471 | acre |
| square kilometer (km2) | 247.1 | Acre |
| square kilometer (km2) | 0.3861 | square mile (mi2) |
| Volume | | |
| cubic meter (m3) | 35.31 | cubic foot (ft3) |
| Flow rate | | |
| cubic meter per second (m3/s) | 35.31 | cubic foot per second (ft3/s) |

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

°F=(1.8×°C)+32

Temperature in degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C=(°F-32)/1.8

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# Introduction

## General

The PEST Surface Water Utilities are a suite of programs whose primary purpose is to assist in the use of PEST with surface water models; however other useful data-processing functions, independent of the calibration process, can also be carried out by many of them. Surface water models are often characterised by the production of lengthy output files containing one or a number of long time series. The data against which the model is to be calibrated is also often voluminous. Because of the amount of data involved, automation of model post-processing tasks and PEST input file preparation is a necessity.

The principal member of the Surface Water Utility suite is TSPROC. In fact, use of TSPROC makes use of some of the other utilities redundant. Nevertheless, all of the original utility programs have been retained within the PEST Surface Water Utility suite, for they may still prove useful in many modelling contexts (especially programs such as SCEUA\_P and PD\_MS2 which can be used as an alternative to PEST, and as an enhancement to PEST respectively in many calibration contexts). However the importance of TSPROC is reflected in the fact that documentation for this program occupies the bulk of this manual, documentation for the other utility programs being assigned to Appendix A.

Appendix B describes the format of a "site sample file", an ASCII file used by many of the programs described herein for the storage of time series data. The format of this file is such that it can be easily exported from, or imported to, a user’s project database, if not directly, then with minimal alterations using a standard text editor.

While most of the programs documented herein are quite general, pertaining to no model in particular, a number are specific to certain models. These model-specific programs transform model output data written in model-specific format to the format required by the utility programs documented herein. Where such a data interface is not provided for a surface water model of particular interest to a specific user, an interface will have to be written by the user him/herself; this is unlikely to be a difficult task. Once this is done, use of PEST with that model can be easily accomplished using the programs documented herein. Alternatively, contact Watermark Numerical Computing; I may be able to write the interface for you.

## Installation Instructions

Copy file swutils.exe (a self-extracting archive) to a suitable directory on your hard disk (eg. c:\swutils). Then run it by tying its name at the command-line prompt. Once the program files have been extracted, you can delete swutils.exe to save disk space. Then edit file autoexec.bat, adding the name of the utilities’ directory to the path environment variable and restart your machine.

## Source Code and Compilation Details

Source code can be provided for all of the PEST Surface Water Utilities on request. All of the Utilities are written in (almost) ANSI Standard FORTRAN 90; thus, theoretically, they can be compiled to run on any platform for which a FORTRAN 90 compiler is available.

## Date Format

For programs other than TSPROC (ie. for all of the older programs documented in Appendix A), a particular file named a "settings file", must reside in the directory from they are run. This file must be named settings.fig. If a settings file is not present in the working directory, these programs will terminate execution with an appropriate error message.

The presence of a settings file is essential for these older members of the Surface Water Utility suite in order that that they know how to read and write date and time information. Depending on the information contained in the settings file, dates are read and written using either the dd/mm/yyyy convention or the mm/dd/yyyy convention. The figure below shows a settings file. The format of this file is obvious from this example; it can be written using any text editor.

date=mm/dd/yyyy

A settings file.

Program TSPROC also needs to know what protocol to use for reading and writing dates. However for TSPROC this information is supplied through its SETTINGS block. Hence the settings file settings.fig does not need to be present in the directory from which it is run.

Other File Formats

See Appendix B for the format specifications of a site sample file and a site listing file.

# Introduction to TSPROC

## General

TSPROC fills two roles. First, it is a time series processor, having the ability to perform many different types of operations on observed and model-generated time series. Second, it automates the generation of PEST input files for calibration tasks of arbitrary complexity based on these time series.

In contrast to the functionality available through other time series analysis software, many of the operations performed by TSPROC are designed specifically for use in the model calibration context. A key element of the processing required in this context is the temporal interpolation of a model-generated time series to the times at which measurements constituting a measurement time series were made. Because measurements of a particular environmental quantity are often intermittent rather than regular, TSPROC does not assume that any individual time series which it manipulates has a constant sample interval. In some instances the absence of this simplifying assumption makes computations carried out by TSPROC a little more inefficient than if time series of constant sample interval were processed. However it does mean that most of the operations carried out by TSPROC are perfectly general in nature.

While TSPROC can be run as an independent executable program, it is also designed to be run as part of a "composite model" by PEST. A "composite model" is a model comprised of two or more executable programs run in succession through a batch or script file. When used in this way TSPROC acts as a model post-processor, carrying out operations of arbitrary complexity on one or many of the time series generated by the model. Similar operations can be carried out on time series comprised of measurement data. The processed measurements and their model-generated counterparts can then be compared, and the discrepancies between the two reduced to a minimum as part of the calibration process undertaken by PEST. In order to facilitate the use of PEST in this context, TSPROC can generate PEST input files appropriate to the type of time series processing that it undertakes as part of the composite model calibrated by PEST.

By using TSPROC it is possible to incorporate some or all of the following data types into the model calibration process:

1. **Raw data** such as flow and constituent measurements. Thus field measurements can be compared directly with their model-generated counterparts after the latter have been interpolated to field measurement times.
2. **Processed data** such as high-pass and low-pass filtered flow time series. TSPROC includes digital filtering capabilities which allow the separation of high, medium and low frequency components of any time series. This can be useful in baseflow separation; see Nathan and McMahon . Modeled and observed filtered counterparts can be individually matched through the calibration process.
3. **Accumulated volumes and masses.** Using TSPROC, flow volumes and constituent masses can be accumulated between any number of arbitrary dates and times occurring within the model simulation period. It has been found that inclusion of volumetric and mass data, calculated on the basis of field measurements on the one hand and model-generated flows and constituent concentrations (interpolated to field measurement times) on the other hand, can bring numerical stability to the parameter estimation process, and result in more robust estimates of parameter values.
4. **Exceedence-time characteristics.** As with volumetric and mass data, inclusion of exceedence-time characteristics in the inversion process can decrease the likelihood of numerical instability at the same time as it promotes estimation of a realistic set of parameter values. Furthermore, in many modelling applications it is crucial that a model predict exceedence-time characteristics as accurately as possible under future climatic/management conditions. A necessary (though not sufficient) condition for achieving this is that the model replicate these characteristics under historical climatic/management conditions; the latter condition is ensured by including these characteristics in the model calibration process.
5. **Summary statistics** and **period statistics** (mean, sum, maximum, minimum, range and standard deviation) calculated from the terms of a time series (or functions of these terms) over varying time intervals. Such items as these can be included in the parameter estimation process in their own right (where statistics calculated on the basis of an observed time series are matched with statistics calculated on the basis of the model-generated counterpart to the observed time series), or can be used in conjunction with PEST’s predictive analyser. For example, in the latter capacity PEST might be asked to maximise or minimise the maximum value of a possible flow or constituent event, while ensuring that model parameters are such that the model remains in a calibrated state.
6. **Functions of arbitrary complexity** calculated on the basis of one or more measured or modeled time series. In many instances of model calibration it may be better to include a comparison of "derived time series", rather than "raw time series" in the parameter estimation process. To achieve this, TSPROC allows the user to calculate any number of new time series based on relationships of arbitrary complexity between existing time series. For example, in some calibration contexts it may be beneficial to compare the log (or some other function) of a measurement type with its model-generated counterpart over all or part of the model simulation time. Or it may be useful to compare a combination of today’s and yesterday’s flow with the model-generated equivalent of this same quantity. Minimising the discrepancies between two such "composite time series" may result in better parameter estimates, as well as better estimates of the uncertainties associated with these parameters, because it incorporates the correlation structure of flow and constituent measurements into the parameter estimation process; see, for example, (Kuczera, 1983).
7. **Data patterns** pertaining to observed time series and their model-generated counterparts. Due to the noisy and erratic nature of some types of environmental measurements (particularly those pertaining to some aspects of water quality), it may not be possible to calibrate a model by attempting to directly match field data with their model-generated counterparts. In such situations it may be better to match relationships between flow and constituent data calculated on the basis of measurements, with identical relationships calculated on the basis of model outputs. Relationships such as those used by the USGS LOADEST program (Runkel and others, 2004) may be suitable in many instances. Implementation of such pattern- or relationship-matching in the parameter estimation process can be accommodated through the use of TSPROC.

## Model Calibration using TSPROC

Inclusion of the above (and many other) types of "processed" data in the calibration process is achieved through carrying out the following steps.

1. Process various types of measurement data to generate an appropriate "value-added measurement dataset".
2. Time-interpolate "raw" model-generated time series to the times at which field measurements were made; then process that data in an identical fashion to that in which the measurement data were processed.
3. Generate a PEST input dataset; this is comprised of a PEST control file recording the value-added measurements used in the calibration process, and an instruction file capable of reading the model-generated counterparts to these "measured" quantities from the appropriate model output file.

The first of the above steps is easily carried out using TSPROC. As presently coded, TSPROC can read field measurements from either a WDM file or from a "site sample file" (see Appendix B). The second of the above operations can be carried out just as easily, provided model-generated time series are recorded in either of these two file formats. Note, however, that TSPROC can also read model-generated time series from a HSPF PLOTGEN file.

As mentioned above, when a model is being calibrated by PEST, TSPROC should be run following the model as part of a batch or script file run by PEST as a "composite model". Hence the "model output file" in this case will, in fact, be a TSPROC output file. This file will contain the model-generated equivalents of the processed field measurements produced through the first of the above steps. The role of the calibration process is then to minimise the discrepancies between these two data sets.

TSPROC can also be used to carry out the third of the above tasks. If provided with the set of template files pertinent to the current calibration exercise (these carrying the names of the parameters to be adjusted through the parameter estimation process), TSPROC will write a complete PEST control file in which these parameters are recorded, together with the (processed) measurements to which model-generated equivalents must be matched through the parameter estimation process. In doing this, TSPROC will assign names to all observations involved in the parameter estimation process, and assign weights to these observations according to formulas of arbitrary complexity supplied by the user; a different formula can be supplied for each measurement type. TSPROC will then write the instruction file by which PEST can read the model-generated equivalents to these (processed) measurements from a TSPROC output file when the latter is run as part of a composite model by PEST.

As can be seen from this brief description, TSPROC is a program of considerable complexity. It was written in order to provide a tool by which most of the arduous data-handling tasks required to calibrate a surface water model can be carried out automatically, thus making PEST setup relatively easy in this context. Furthermore, its design is such as to allow a large degree of flexibility in the way this process is carried out, thus allowing a modeller to tailor the parameter estimation process to the demands of his/her particular modelling application. As time goes on, and as more experience is gained in applying PEST to surface water model calibration, the functionality included in TSPROC will be increased accordingly. This is only the beginning.

# Using TSPROC

## Running TSPROC

TSPROC is run by typing its name at the screen prompt. TSPROC prompts for only two items of information. The first is the name of its input file; the second is the name of its run record file. The TSPROC input file contains all of the information required for TSPROC to perform the various operations for which it was designed. As it carries out these operations it echoes the contents of its input file, and the operations that it performs in response to the instructions provided in that file, to the screen and to its run record file. A TSPROC input file is easily prepared using a text editor.

If TSPROC is requested to generate a set of PEST input files it will prompt the user before overwriting any existing files of the same name. For example, it may prompt:

File instruct.ins already exists. Overwrite it? [y/n]:

Type "y" or "n", followed by <Enter> as appropriate. Note that TSPROC does not prompt in this manner when overwriting data files as part of its time series manipulation functionality. This is because, if it is run many times in the course of a PEST run, such files will need to be overwritten on each occasion that it is run. However if the user forgets to de-activate instructions within a TSPROC input file for generation of PEST input files (see below) before TSPROC is used by PEST in a parameter estimation run, then the above warning message may save previously-generated PEST input files (perhaps those being used for the current PEST run) from being overwritten.

If TSPROC is run by PEST as part of a composite model, then the responses to TSPROC’s prompts must be placed into a text file prior to the PEST run and provided to TSPROC through the command-line re-direction mechanism. For example, if it is desired that TSPROC read an input file named tsproc.dat and that it record details of its operations to a run record file named tsproc.rec, then a text file (named, for example, tsproc.in) should be prepared with its contents as follows:-

1. Contents of a text file containing the responses to TSPROC prompts.

tsproc.dat

tsproc.rec

When TSPROC is then run as part of a composite model by PEST, the pertinent line in the composite model batch file should be:

1. Example command line for starting a TSPROC run.

tsproc < tsproc.in

(The "<" symbol instructs TSPROC to look for its keyboard input from the ASCII file whose name follows it.) Of course the above command can be issued from the keyboard as well if file tsproc.in has already been prepared.

Because TSPROC is a complex program which carries out many different types of operations, its input file must be carefully and thoughtfully prepared. It is not impossible that a user will make an error in preparation of this file. Should this occur, TSPROC will report the error to the screen, and to its run record file, and then cease execution; it will not read its input file any further, nor perform any operations beyond that at which the error occurred. Thus while TSPROC’s error-checking functionality is quite comprehensive, it will only find one error at a time in a TSPROC input file that contains multiple errors.

In some circumstances a user may desire that TSPROC not report its activities to the screen, for example if TSPROC is being run under the control of PEST and the user wishes that TSPROC screen output not interfere with that of PEST. As with any command-line program, TSPROC output can be re-directed from the screen to a file, thus leaving the screen bare. Because the TSPROC run record file contains all of the information that TSPROC writes to the screen, there is nothing to be gained through keeping such a file which contains re-directed screen output; hence it is best to re-direct TSPROC screen output to the "nul" file, (ie. to nowhere). Hence if it is desired that TSPROC look to a file named tsproc.in for its keyboard input, and that it re-direct its screen output to the "nul" file, it should be run using the command:

tsproc < tsproc.in > nul

## The TSPROC Input File - Overview

The TSPROC input file is divided into a series of sections or "blocks". Within each block, various items of information are supplied following pertinent "keywords" which identify each such item. In most blocks these keywords can be supplied in any order; however there are some exceptions to this rule which will be pointed out in the pertinent sections of this manual. (TSPROC will also inform you, through an appropriate error message, if keyword ordering is incorrect.) Keywords are shown capitalised in the illustrations used throughout this document for ease of recognition. Note, however, that the contents of a TSPROC input file are case-insensitive.

Any line within a TSPROC input file beginning with the "#" character is ignored. Thus comments can be freely interspersed with data elements in a TSPROC input file. The complex nature of the instructions that can be supplied to TSPROC through its input file makes the inclusion of comments in this file a good idea.

1. Example of a TSPROC input file.

START SETTINGS

CONTEXT pest\_input

DATE\_FORMAT mm/dd/yyyy

END SETTINGS

####################################################################

# Modeled river flows are read from a HSPF output file.

####################################################################

START GET\_SERIES\_PLOTGEN

CONTEXT all

FILE catchment.plt

LABEL "total outflow"

NEW\_SERIES\_NAME flow\_mod

END GET\_SERIES\_PLOTGEN

####################################################################

# Observed river flows are read from a WDM file.

####################################################################

START GET\_SERIES\_WDM

CONTEXT all

FILE catchment.wdm

DSN 113

NEW\_SERIES\_NAME flow\_obs

END GET\_SERIES\_WDM

####################################################################

# Modeled flows are interpolated to the times of observed flows.

####################################################################

START NEW\_TIME\_BASE

CONTEXT all

SERIES\_NAME flow\_mod

TB\_SERIES\_NAME flow\_obs

NEW\_SERIES\_NAME i\_flow\_mod

END NEW\_TIME\_BASE

####################################################################

# Flow volumes are accumulated for the modeled time series.

####################################################################

START VOLUME\_CALCULATION

CONTEXT all

SERIES\_NAME i\_flow\_mod

NEW\_V\_TABLE\_NAME vol\_mod

FLOW\_TIME\_UNITS days

DATE\_FILE dates.dat

END VOLUME\_CALCULATION

####################################################################

# Flow volumes are accumulated for the observed time series.

####################################################################

START VOLUME\_CALCULATION

CONTEXT pest\_input

SERIES\_NAME flow\_obs

NEW\_V\_TABLE\_NAME vol\_obs

FLOW\_TIME\_UNITS days

DATE\_FILE dates.dat

END VOLUME\_CALCULATION

####################################################################

# Exceedence times are calculated for the modeled time series.

####################################################################

START EXCEEDENCE\_TIME

CONTEXT all

SERIES\_NAME i\_flow\_mod

NEW\_E\_TABLE\_NAME time\_mod

EXCEEDENCE\_TIME\_UNITS days

FLOW 0

FLOW 10

FLOW 20

FLOW 50

FLOW 100

FLOW 200

END EXCEEDENCE\_TIME

####################################################################

# Exceedence times are calculated for the observed time series

####################################################################

START EXCEEDENCE\_TIME

CONTEXT pest\_input

SERIES\_NAME flow\_obs

NEW\_E\_TABLE\_NAME time\_obs

EXCEEDENCE\_TIME\_UNITS days

FLOW 0

FLOW 10

FLOW 20

FLOW 50

FLOW 100

FLOW 200

END EXCEEDENCE\_TIME

####################################################################

# Modeled time series and tables are written to a file.

####################################################################

START LIST\_OUTPUT

CONTEXT all

FILE model.out

SERIES\_NAME i\_flow\_mod

V\_TABLE\_NAME vol\_mod

E\_TABLE\_NAME time\_mod

SERIES\_FORMAT short

END LIST\_OUTPUT\_BLOCK

####################################################################

# PEST input files are written.

####################################################################

START WRITE\_PEST\_FILES

CONTEXT pest\_input

NEW\_PEST\_CONTROL\_FILE case.pst

TEMPLATE\_FILE catchment.tpl

MODEL\_INPUT\_FILE catchment.uci

TEMPLATE\_FILE extra.tpl

MODEL\_INPUT\_FILE extra.dat

NEW\_INSTRUCTION\_FILE observation.ins

AUTOMATIC\_USER\_INTERVENTION yes

########### Time series observations ######

OBSERVATION\_SERIES\_NAME flow\_obs

MODEL\_SERIES\_NAME i\_flow\_mod

SERIES\_WEIGHTS\_EQUATION 1.0/sqrt(@\_abs\_value)

SERIES\_WEIGHTS\_MIN\_MAX 1.0 100.0

############# volumes ######################

OBSERVATION\_V\_TABLE\_NAME vol\_obs

MODEL\_V\_TABLE\_NAME vol\_mod

V\_TABLE\_WEIGHTS\_EQUATION 5.0

############# exceedence-times #############

OBSERVATION\_E\_TABLE\_NAME time\_obs

MODEL\_E\_TABLE\_NAME time\_mod

E\_TABLE\_WEIGHTS\_EQUATION log(2.0/@\_abs\_value) + 2.0

E\_TABLE\_WEIGHTS\_MIN\_MAX 0 1000

############ other data ####################

PARAMETER\_DATA\_FILE param.dat

END WRITE\_PEST\_FILES

Each block within a TSPROC input file instructs TSPROC to carry out a certain type of operation. Information supplied within a block informs TSPROC of the names of the entities to be processed, and the names of the entities to be produced as a result of that processing. Any other information required by TSPROC to enable that processing to take place is also supplied within the block through the appropriate keyword. For each block some keywords are optional and some are mandatory. Where an optional keyword is not supplied TSPROC supplies a default value for its associated variable.

With one exception (see below) blocks can be arranged in a TSPROC input file in any order. However because TSPROC processes blocks in the order in which they are supplied, the ordering of blocks can be important in many applications (for example if an entity that is produced in one block is used by another block).

## The DATE\_FORMAT and CONTEXT Settings

In any TSPROC input file, there is one block which must be present, and which must precede all other blocks. This is the SETTINGS block. The SETTINGS block must contain two keywords, viz. the DATE\_FORMAT and CONTEXT keywords.

The DATE\_FORMAT keyword informs TSPROC of the protocol to be used for representation of dates in all input files which it reads and output files which it generates. Only two options are presently available viz. dd/mm/yyyy and mm/dd/yyyy.

The CONTEXT keyword must be followed by a character string of 20 characters or less (with no embedded spaces) which "sets the context" for the current TSPROC run. A CONTEXT keyword is also a mandatory element of every other block appearing in a TSPROC input file; as in the SETTINGS block, the CONTEXT keyword in all of these blocks must be followed by a string of 20 characters or less. Up to five CONTEXT keywords can appear in any TSPROC processing block. (A "processing block" is any block other than the SETTINGS block.) If the CONTEXT string following any of the CONTEXT keywords in a processing block agrees with that in the SETTINGS block, then the instructions in that block will be implemented by TSPROC. If not, they will be ignored (unless at least one of the CONTEXT strings supplied in a processing block is "all", in which case the operations listed in the block will be carried out regardless of the current TSPROC context as defined in the SETTINGS block). Furthermore CONTEXT keywords must precede all other keywords in the block. Use of the CONTEXT concept allows a user to "turn on" and "turn off" various processes cited in a TSPROC input file, simply by altering the CONTEXT string in the SETTINGS block. This can be very useful when preparing for a PEST run.

## Blocks within a TSPROC Input File

The following table lists the blocks which may be present within any TSPROC input file. Multiple occurrences of any block except the SETTINGS block are permitted.

1. TSPROC input blocks.

## Blocks occurring within a TSPROC input file.

Most of the tasks carried out by TSPROC are related to the processing of time series. As stated above, these time series may, or may not, be of constant sample interval. A time series can be comprised of as little as one sample, or as many as tens of thousands of samples.

Each time series must be given a name by the user when it is imported into TSPROC or produced as an outcome of the processing encapsulated in a TSPROC processing block; a time series is normally named using a NEW\_SERIES\_NAME keyword. A time series name must be 10 characters or less in length.

At first sight it might appear that 10 characters is unduly restrictive for the name of a time series. The reason for this restriction in length is based on the fact that observation and observation group names used in a TSPROC-generated PEST control file must be formed from the names of these TSPROC entities. For lengthy time series, observations can number in the tens of thousands; TSPROC creates observation names by appending the time series term number to the time series name, or a contraction of the time series name if appropriate. The chances of observation name nonuniqueness are considerably reduced if time series names are restricted to 10 characters in length within TSPROC, thus requiring that the user maintain uniqueness in nomenclature at the 10 character level. Nevertheless, should duplicate observation names be created as a result of its name formation process, TSPROC will detect this and generate an appropriate error message. If the shortness of a time series name prevents an adequate characterisation of the source of each time series, the user is advised to tabulate the hereditary of each time series on a piece of paper.

Many of the processing options provided by TSPROC produce a new time series through the processing or manipulation of one or a number of existing time series. Where this occurs the user must provide the name of both the existing time series (through a SERIES\_NAME keyword) and the new time series (through a NEW\_SERIES\_NAME keyword) to the processing block through which the operation is being undertaken.

Sometimes the processing of a time series results in the creation of an entity which is not another time series. When TSPROC calculates certain statistics pertaining to the terms of a time series (through the SERIES\_STATISTICS block), these statistics are stored in an "s\_table". The outcomes of volumetric calculations carried out by the VOLUME\_CALCULATION block are stored in a v\_table. The outcomes of exceedence time calculations carried out by the EXCEEDENCE-TIME block are stored in an e\_table. Statistics based on the comparison of two time series are written to a "c\_table". Like the time series entity, each of these other entities must be assigned a name of 10 characters or less in length, this name being provided by the user following the NEW\_C\_TABLE, NEW\_S\_TABLE, NEW\_V\_TABLE and NEW\_E\_TABLE keywords in the pertinent processing blocks. More entities will probably be added to TSPROC over time as the need arises.

TSPROC will never overwrite one entity with another. Hence the name provided for a new entity in a processing block must be different from the name of any existing entity of the same type. If desired, entities can be erased from memory in order to make room for other entities using the ERASE\_ENTITY block. This functionality can be very important when processing lengthy time series which make large demands on computer memory.

Each TSPROC block is now discussed. Descriptions are arranged in alphabetical order.

## DIGITAL\_FILTER

The DIGITAL\_FILTER block instructs TSPROC to calculate a new time series from an existing time series by passing the latter through a digital filter. Two types of filter are provided. The Butterworth filter can remove high frequency components (low pass filter), low frequency components (high pass filter), or both of these (band pass filter) from the original time series. The "baseflow separation" filter allows extraction of quick response from a flow time series; baseflow can then be obtained by subtraction from the original series using the SERIES\_EQUATION block.

The nature of digital filtering is such that it can only be performed on a time series for which the sample interval is constant. Thus before performing filtering operations TSPROC checks the nominated time series for this condition; if it is not met, TSPROC terminates execution with an error message. (Use the NEW\_TIME\_BASE block in conjunction with the NEW\_SERIES\_UNIFORM block to create a time series interpolated to a uniform time base if this is a problem.)

Keywords available in the DIGITAL\_FILTER block are listed in the following table. Two examples of a DIGITAL\_FILTER block follow that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a DIGITAL\_FILTER block.
2. Example usage of a DIGITAL\_FILTER block for use in applying a Butterworth filter.

START DIGITAL\_FILTER

CONTEXT context\_1

FILTER\_TYPE butterworth

SERIES\_NAME flow

NEW\_SERIES\_NAME av\_flow

FILTER\_PASS low

CUTOFF\_FREQUENCY 0.08

END DIGITAL\_FILTER

1. Example usage of a DIGITAL\_FILTER block for use in applying a baseflow\_seperation filter.

START DIGITAL\_FILTER

CONTEXT context\_1

FILTER\_TYPE baseflow\_separation

SERIES\_NAME flow

NEW\_SERIES\_NAME qflow

ALPHA 0.95

PASSES 1

CLIP\_INPUT yes

CLIP\_ZERO yes

END DIGITAL\_FILTER

Digital filtering is a fast and powerful means of accentuating certain aspects of a time series and removing others. A high pass filter removes long-term variations from a time series, while a low pass filter removes short term variations. A band pass filter removes both short and long-term variations, allowing only medium-term variations to remain in the filtered time series. Many different types of filters can be constructed to implement all three of these types of operation. TSPROC implements the Butterworth filter; this has the desirable property that its frequency response is maximally flat within the pass band. It also implements a "baseflow separation" filter – a form of high pass filter with a more gentle frequency rolloff than the Butterworth filter outside the pass band. This is suitable for separation of the quickflow component of streamflow; baseflow can then be obtained by subtraction from the original streamflow. See Nathan and McMahon for details.

Frequencies within the pass band of a filter are conveyed with minimal attenuation. However as the edge of the pass band is approached, and outside the passband, attenuation of the input time series takes place. The diminution of output amplitude with increasing or decreasing frequency outside the passband is referred to as "rolloff" in filtering jargon. The more stages that a filter employs, the steeper is this rolloff. However steep rolloff comes at a price – this being the tendency for the filter output to oscillate or "ring" in response to high amplitude events within the input time series. A phase delay between the input and output time series can also be introduced. For a 1-stage Butterworth filter the rolloff is 6db/octave; for a 2-stage Butterworth filter it is 12 db/octave, while for a 3-stage Butterworth filter it is 18 db/octave. Rolloff is 3db/octave for one pass of the baseflow separation filter, and 9db per octave for 3 passes of this filter. An octave is a doubling of frequency; a db is a measure of signal power gain or loss. A rolloff rate of 6db/octave is equivalent to a halving of output amplitude with every factor of two change in frequency. (This is sufficient, or more than sufficient, for most applications in surface water hydrology.)

Use of each of the types of digital filter implemented by TSPROC is now discussed in detail.

### Butterworth Filter

When using a Butterworth filter, the frequency characteristics of the filter must be provided directly through pertinent keywords within the DIGITAL\_FILTER block.

The boundary between the passband and the stopband of a filter is normally denoted by the "3db point". This is the frequency at which the amplitude response is a factor of about √2 less than it is in the pass band. In designing a low pass Butterworth filter, one such frequency is required; this is supplied with the CUTOFF\_FREQUENCY keyword. The same holds for a high pass Butterworth filter, except that the amplitude rolls off with decreasing frequency from the 3db point for a high pass filter whereas it rolls off with increasing frequency from the 3db point for a low pass filter. For a band pass filter an upper and lower 3db frequency are required. These must be supplied following the CUTOFF\_FREQUENCY\_1 and CUTOFF\_FREQUENCY\_2 keywords. The former must be less than the latter or TSPROC will terminate processing of the DIGITAL\_FILTER block with an appropriate error message.

Frequencies must be supplied in units of day-1 no matter what the time increment of the time series. Sometimes it is easier to think in terms of period rather than frequency; period is the reciprocal of frequency. A fluctuation which repeats itself every n days has a frequency of 1/n day-1. n can be greater or less than a day. For a period of 6 hours n is ¼ days and the frequency is 4 day-1; for a period of 10 days, the frequency is 1/10 day-1.

A high, low or band pass cutoff frequency must be less than one half the sample frequency of the time series which is undergoing filtering. Thus, for example, a cutoff frequency for an hourly time series must be less than 12 day-1. A cutoff frequency for a daily time series must be less than 0.5 day-1.

As mentioned above, steeper frequency rolloff can be achieved through using more than one filter STAGE; up to three STAGEs are allowed by TSPROC. However if a STAGE keyword is not supplied, a single stage is assumed. While more stages mean greater signal rejection within the frequency stopband, the resulting propensity for "ringing", and the greater phase lag between the input and output signals, may be unwanted in many hydrologic applications.

### Baseflow Separation Filter

Only two keywords are required to specify the characteristics of a baseflow separation filter. These are the ALPHA and PASSES keywords. ALPHA is the rate of decay of baseflow relative to current flow rate; a value of 0.92 to 0.98 is suitable for most applications; however as pointed out by Nathan and McMahon , a little trial and error may be required for selection of the most appropriate value for any particular application. Its value is independent of the series sample interval. PASSES is similar to the STAGE keyword required by the Butterworth filter. However it is also a little different in that, unlike the Butterworth filter, different internal filter coefficients are not used for different passes. Furthermore, only 1 or 3 passes can be implemented, with the second pass being implemented in the reverse direction to mitigate phase shifts. If the PASSES keyword is not supplied, a value of 1 is assumed.

The outcome of implementation of a baseflow separation filter is a time series which represents the "quick response" streamflow. Baseflow can then be obtained by subtracting this from the original streamflow time series using the SERIES\_EQUATION block. Occurrence of subzero filtered terms, or terms which are greater than the original streamflow record, can be prevented by clipping – see below.

### Clipping

The outputs of the baseflow separation filter (but not the Butterworth filter) can be clipped in order to prevent the occurrence of negative values, or of values which are greater than those of the input time series. Sub-zero values can be prevented using the CLIP\_ZERO keyword, and values which are higher than the input time series can be prevented using the CLIP\_INPUT keyword; in either case a "yes" or "no" specifier must be provided in the DIGITAL\_FILTER block. A default of "no" is assumed in either case. Clipping is often very useful in conjunction with baseflow separation filtering. It should be remembered, however, that the action of this filter is to provide time series which have similar characteristics to baseflow and quickflow. This, indeed, can be extremely helpful in calibration of a model where the contribution of both of these to the objective function can be monitored (and enhanced if desired through appropriate weights selection). However it should not be forgotten that the calibrated model is then likely to produce a better quickflow/ baseflow time series than the digital filter used to assist in the calibration process.

### Settling Time

You should be aware of the fact that a filter sometimes takes a while to "settle down" when filtering operations begin on a time series. This will apply more to a multi-stage Butterworth filter than to the other filter types implemented by TSPROC. To ensure integrity of a filtered time-series it may sometimes be necessary to remove the first part of the series using the REDUCE\_TIME\_SPAN block. Note also, that TSPROC will not allow filtering operations to take place on any time series that has fewer than 20 entries.

As mentioned above, filtering can only be implemented on a time series in which the sample interval is constant throughout the series. TSPROC will report any attempt to filter a time series with non-constant sample interval.

### Reverse Filtering

If FILTER\_TYPE is set to "butterworth", FILTER\_PASS is set to "low" and STAGES is set to 2, the second stage of Butterworth filtering can be performed in the reverse direction to that of the first stage of filtering. Low pass filtering can incur a substantial phase shift, thereby delaying peaks and troughs occurring within the original time series. This phase-change-induced delay can be rectified by running the digital filter from late times to early times in the second filtering stage.

The user should use this option with caution. It can sometimes actually amplify the low-frequency component of filtered peaks and troughs remaining after the two-stage filtering operation has taken place.

## ERASE\_ENTITY

If a time series, c\_table, s\_table, v\_table or e\_table is no longer required by TSPROC, it can be erased from TSPROC’s memory in order to make room for other TSPROC entities. This may be a wise thing to do if a time series which contains many terms is no longer required. This is achieved through use of the ERASE\_ENTITY block. Keywords found in the ERASE\_ENTITY block are listed in the table below; an example of an ERASE\_ENTITY block follows that.

Keywords in the ERASE\_ENTITY block can be supplied in any order except for the CONTEXT keyword(s), which must precede all other keywords.

1. Keywords in an ERASE\_ENTITY Block.
2. Example usage of a ERASE\_ENTITY block.

START ERASE\_ENTITY

CONTEXT context\_1

C\_TABLE\_NAME compare

E\_TABLE\_NAME ex\_flow

S\_TABLE\_NAME stat\_flow

V\_TABLE\_NAME vol\_flow

SERIES\_NAME flow

END ERASE\_ENTITY

## EXCEEDENCE\_TIME

The EXCEEDENCE\_TIME block instructs TSPROC to calculate the time over which user-supplied flows or fluxes have been exceeded, or over which such nominated flows or fluxes have not been exceeded. The outcomes of EXCEEDENCE\_TIME calculations are stored in an e\_table. Like every other storage entity used by TSPROC, the user must provide a name for each e\_table produced in this manner so that it can be referenced in later processing.

Keywords available in the EXCEEDENCE\_TIME block are listed in the following table; an example of an EXCEEDENCE\_TIME block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others, and the DELAY keyword which (if used) must directly follow a FLOW keyword.

1. Keywords in an EXCEEDENCE\_TIME block.
2. Example usage of a EXCEEDENCE\_TIME block.

START EXCEEDENCE\_TIME

CONTEXT all

SERIES\_NAME outflow

NEW\_E\_TABLE\_NAME et\_flow

EXCEEDENCE\_TIME\_UNITS days

FLOW 0.0

FLOW 10.0

FLOW 20.0

FLOW 50.0

FLOW 100.0

FLOW 200.0

END EXCEEDENCE\_TIME

Any number of FLOW keywords can be provided in an EXCEEDENCE\_TIME block. For each such FLOW, if UNDER\_OVER is set to "over" (or if this keyword is omitted) and if no DELAY keywords are supplied, TSPROC calculates the accumulated time over which the nominated flow was exceeded. Alternatively, if UNDER\_OVER is set to "under", TSPROC calculates the accumulated time for which flow was less than each nominated FLOW. Note that in carrying out these calculations TSPROC does more than simply count the number of time series terms which exceed, or are less than, the value of each FLOW, and then multiply the number of terms by the series sampling interval. This would be an incorrect procedure for two reasons. The first of these reasons is that, as mentioned above, TSPROC does not assume a uniform sampling interval for any series. The second reason is that an exceedence-time calculation that is carried out in this way on the basis of a model-generated time-series will be slightly discontinuous with respect to model parameters (which will lead to a degradation in the performance of PEST as it attempts to estimate these parameters). Instead, TSPROC carries out linear interpolation between the terms of a time series to find the "exact time" at which a FLOW threshold was crossed, and commences or ceases time-accumulation from that point. The result is a continuous relationship between exceedence times and parameters as the latter vary during a parameter estimation process.

Exceedence times calculated by TSPROC can be stored internally (and listed through the LIST\_OUTPUT block) in time units of years, months, days, hours, minutes or seconds. The user must choose one of these options through the mandatory EXCEEDENCE\_TIME\_UNIT keyword.

Note that exceedence time calculations carried out by TSPROC need not be limited to time series which represent flow. A suitable time series could represent any environmental quantity; the numbers following the FLOW keywords in the EXCEEDENCE\_TIME block would then refer to the same quantity.

Use of the DELAY keyword requires special consideration. An EXCEEDENCE\_TIME block in which this keyword is featured is shown below.

1. Example of an EXCEEDENCE\_TIME block showing the use of the DELAY keyword.

If a DELAY keyword is used, it must directly follow the FLOW keyword to which it pertains. Furthermore a DELAY keyword must follow all FLOW keywords, or follow none at all.

Use of the DELAY keyword controls the way in which exceedence time is accumulated over the period spanned by a time series. In the example shown above, UNDER\_OVER is set to "under". Hence, for the first FLOW entry (viz. 20), time over which elements of the "sim\_flow" series are less than 20 is accumulated. However, for any one "below 20" event, time accumulation does not begin until 3 days after the beginning of the event; the time units pertaining to the DELAY keyword are assumed to be those supplied with the EXCEEDENCE\_TIME\_UNITS keyword. Thus the total exceedence time calculated by TSPROC for the flow of 20 will actually be the total time for which the flow was less than 20, but which was preceded by an interval of at least 3 days for which the flow was also less than 20.

Use of the DELAY keyword can be particularly useful when studying the effect of stream condition on biotic health. In many instances, the lethality of a particular adverse condition is a function of the magnitude of the condition and the duration over which the condition prevails. The more harmful the condition, the shorter the time which elapses before the condition exerts a deleterious influence on system health. This relationship is often described by "toxicity curves" relating, for example, concentration of a constituent to the exposure time. The greater is the concentration, the less is the exposure time required to cause damage.

By accumulating the time over which a user-specified chemical concentration or sediment load is exceeded (or for which flow is below a user-specified threshold), and by subtracting the time required for the onset of harmful effects during each such "toxicity event", the total time over which biotic health suffered can be calculated. This may be an extremely useful model prediction, and one to which PEST’s predictive analysis capabilities may be fruitfully turned.

If a user desires that EXCEEDENCE\_TIME calculations be restricted to a certain date/time interval, a time series can be shortened prior to EXCEEDENCE\_TIME calculations using the REDUCE\_TIME\_SPAN block.

## GET\_MUL\_SERIES\_GSFLOW\_GAGE

The GET\_MUL\_SERIES\_GSFLOW\_GAGE block is used for extracting one or a number of time series from a "gage file" produced by the USGS GSFLOW model. This model produces two types of gage file, each with a slightly different header format. One of these lists model-calculated quantities pertaining to surface water features including lakes and rivers. The other lists model-calculated quantities computed by the UZ process. In either case, the file is comprised of multiple columns, each of which is associated with a header which specifies the information recorded in the column. One of these columns is elapsed simulation time. Data associated with any of the other columns can be extracted by providing the name of its header.

Keywords available in the GET\_MUL\_SERIES\_GSFLOW\_GAGE block are listed in the following table; an example of a GET\_MUL\_SERIES\_GSFLOW\_GAGE block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a GET\_MUL\_SERIES\_GSFLOW\_GAGE block.
2. Example usage of a GET\_MUL\_SERIES\_GSFLOW\_GAGE block.

START GET\_MUL\_SERIES\_GSFLOW\_GAGE

CONTEXT all

FILE file1a.ggo

DATA\_TYPE flow

NEW\_SERIES\_NAME flow\_s

DATA\_TYPE uzf-runoff

NEW\_SERIES\_NAME uzfr\_s

TIME\_UNITS\_PER\_DAY 1

MODEL\_REFERENCE\_DATE 1/1/2000

MODEL\_REFERENCE\_TIME 12:00:00

DATE\_1 3/4/2005

TIME\_1 12:00:00

DATE\_2 6/9/2010

TIME\_2 00:00:00

END GET\_MUL\_SERIES\_GSFLOW\_GAGE

As for other TSPROC blocks which read multiple time series from the one file, entries pertaining to each imported series must be grouped. Thus one or a number of pairs of DATA\_TYPE and NEW\_SERIES\_NAME keywords (in that order) must be provided in the GET\_MUL\_SERIES\_GSFLOW\_GAGE block. DATA\_TYPE refers to a column header in the GSFLOW gage file, while NEW\_SERIES\_NAME provides the name of the imported series as stored by TSPROC. There is no limit to the number of these keyword pairs that can appear in a GET\_MUL\_SERIES\_GSFLOW\_GAGE block; a new series is imported for each such pair. (Note that DATA\_TYPE is case-insensitive; it will be matched to the pertinent heading in the GSFLOW gage file irrespective of the case employed for representation of this string either in the TSPROC input file, or in the GSFLOW gage file from which the series is imported.)

Each GSFLOW gage file contains a "time" column (with an appropriate header which designates it as such). Entries in this column are normally in days; indeed, unless a TIME\_UNITS\_PER\_DAY keyword is present within the GET\_MUL\_SERIES\_GFLOW\_GAGE block, TSPROC will assume this to be the case. However where the time units are different from days, TSPROC must employ a time conversion factor as it imports the time series, this factor being supplied as the entry following the TIME\_UNITS\_PER\_DAY keyword. Suppose that time units are actually hours; then TIME\_UNITS\_PER\_DAY should be supplied as 24.0. Thus, as the name suggests, it is the number of time units employed by the model which collectively comprise one day.

To convert model simulation time to days and times, a reference date and time is needed, this being the date and time corresponding to a simulation time of zero. These must be supplied following the MODEL\_REFERENCE\_DATE and MODEL\_REFERENCE\_TIME keywords, both of which are mandatory in the GET\_MUL\_SERIES\_GSFLOW\_GAGE block.

The DATE\_1, TIME\_1 and DATE\_2, TIME\_2 keywords can be employed to restrict the length of the time series which is imported into TSPROC. No entries before DATE\_1, TIME\_1 or after DATE\_2, TIME\_2 are imported. Missing TIME\_1 and TIME\_2 entries denote a time of 00:00:00 in each case. Either or both of the DATE\_1 and DATE\_2 keywords can be omitted from the GET\_MUL\_SERIES\_GSFLOW\_GAGE block. If both of them are missing, the entirety of the time series is imported.

## GET\_MUL\_SERIES\_SSF

The role of the GET\_MUL\_SERIES\_SSF block is very similar to that of the GET\_SERIES\_SSF block, the only difference being that multiple series can be imported from a site sample file in one operation using the former block, whereas only one series can be imported using the latter block. See Appendix B for the format of a site sample file. Because a site sample file is used for time series storage by other members of the PEST Surface Water Utilities suite, TSPROC can readily import time series data written by other members of the suite. Also, if it is desired that TSPROC be used in the calibration of a model for which it is presently incapable of directly importing results, then this can be implemented by writing a small translation program which converts the outputs of that model to site sample file format. This program would be run between the model and TSPROC as part of a composite model calibrated by PEST.

The table below shows the keywords appearing in a GET\_MUL\_SERIES\_SSF block. An example of a GET\_MUL\_SERIES\_SSF block is shown following that. Note that the CONTEXT keyword(s) must precede all other keywords cited in this block.

1. Keywords in a GET\_MUL\_SERIES\_SSF block.
2. Example usage of a GET\_MUL\_SERIES\_GSFLOW\_GAGE block.

START GET\_MUL\_SERIES\_SSF

CONTEXT all

FILE flows.smp

SITE rebec\_ck

NEW\_SERIES\_NAME rebecca

SITE horton\_ck

NEW\_SERIES\_NAME horton

SITE sandy\_ck

NEW\_SERIES\_NAME sandy

DATE\_1 06/03/1970

TIME\_1 12:00:00

DATE\_2 09/01/1980

TIME\_1 00:00:00

END GET\_MUL\_SERIES\_SSF

The DATE\_ and TIME\_ specifiers are optional. If they are omitted then the entire time series pertaining to each of the nominated sites is imported. If a DATE\_1 keyword is present but a TIME\_1 keyword is absent, then TIME\_1 is assumed to be 00:00:00; similarly for DATE\_2. If TIME\_1 is present then DATE\_1 must be present; the same holds for TIME\_2.

A GET\_MUL\_SERIES\_SSF block can contain multiple incidences of the SITE and NEW\_SERIES\_NAME keywords. However these must be supplied in pairs with the SITE keyword immediately preceding the pertinent NEW\_SERIES\_NAME keyword. The character string associated with the SITE keyword, must pertain to a site which appears within the nominated site sample file; The same site cannot be supplied twice.

Correct operation of the instructions contained within the GET\_MUL\_SERIES\_SSF block assumes that the site sample file read using this block is correct and consistent. The integrity of a site sample file can be checked with the utility program SMPCHEK supplied with the Surface Water Utility suite.

## GET\_MUL\_SERIES\_STATVAR

STATVAR files are written by the Precipitation-Runoff Modelling System (PRMS) model, as well as by the Modular Modelling System (MMS) model. An example of such a file is provided below.

1. Example of the header and first three lines of a STATVAR file.

4

node\_cfs.musroute 132

runoff.obs 16

node\_cfs.musroute 87

node\_cfs.musroute 14

1 1975 6 1 0 0 0 2.490942 6.434562 3.300000 0.000000

2 1975 6 2 0 0 0 2.501948 7.389743 2.800000 0.000000

3 1975 6 3 0 0 0 2.476184 9.652343 2.900000 0.000000

*{…continues…}*

The STATVAR file begins with the number of series N represented in the file. Following that are N lines, each containing a variable name followed by a "location identifier". Taken together, these uniquely identify a series. Following these N lines are the data comprising the time series themselves. The first entry on each such line is the model simulation day. Following that are the year, month, day, hour, minute and second respectively corresponding to series entries on that line followed by the entries themselves; entries are in the same order as variable name and location id entries provided in the header to the file.

Keywords that can be employed in a GET\_MUL\_SERIES\_STATVAR block are provided in the table below. An example of a GET\_MUL\_SERIES\_STATVAR block follows that.

1. Keywords in a GET\_MUL\_SERIES\_STATVAR block.
2. Example usage of a GET\_MUL\_SERIES\_STATVAR block.

START GET\_MUL\_SERIES\_STATVAR

CONTEXT all

FILE statvar.dat

VARIABLE\_NAME node\_cfs.musroute

LOCATION\_ID 132

NEW\_SERIES\_NAME runoff16

VARIABLE\_NAME node\_cfs.musroute

LOCATION\_ID 2

NEW\_SERIES\_NAME cfs2

DATE\_1 6/4/1975

TIME\_1 12:00:00

DATE\_2 10/29/2001

TIME\_2 00:00:00

END GET\_ MUL\_SERIES\_STATVAR

A GET\_MUL\_SERIES\_STATVAR block can be used to import one or a number of series from a STATVAR file. Each imported series is identified by a VARIABLE\_NAME and LOCATION\_ID. These two keywords must be supplied in that order, immediately followed by a NEW\_SERIES\_NAME keyword for each series to be imported. As many such triplets must be featured in this block as there are series to import.

The DATE\_1, TIME\_1, DATE\_2 and TIME\_2 keywords are optional. If none of these is supplied then the entirety of each time series is imported. If any of these are present, then no series terms which precede DATE\_1, TIME\_1 or postdate DATE\_2, TIME\_2 will be imported. If TIME\_1 or TIME\_2 is omitted, a time of 00:00:00 is assumed in either case.

## GET\_SERIES\_PLOTGEN

The GET\_SERIES\_PLOTGEN block governs importation of time series data from a HSPF PLOTGEN file into TSPROC. There is an important difference between use of this block and use of some of the other blocks which import time series data into TSPROC; when importing data from a PLOTGEN file, more than one time series can be imported using the same block. This saves TSPROC from having to read a HSPF PLOTGEN file many times in order to import multiple time series produced during a HSPF run.

Another slight difference between series importation using the GET\_SERIES\_PLOTGEN block and series importation using other TSPROC blocks is that the ordering of some keywords is important in the GET\_SERIES\_PLOTGEN block. In particular, each NEW\_SERIES\_NAME keyword provided in this block must directly follow a LABEL keyword so that the association between the time series label in the HSPF PLOTGEN file and the name of the new series as stored within TSPROC is clear. Due to the multiple time series importation capabilities of the GET\_SERIES\_PLOTGEN block, more than one of these LABEL/NEW\_SERIES\_NAME pairs can be present within any such block. See the table below.

1. Keywords in a GET\_SERIES\_PLOTGEN block.
2. Example usage of a GET\_SERIES\_PLOTGEN block.

START GET\_SERIES\_PLOTGEN

CONTEXT all

FILE hspfout.plt

LABEL "total outflow"

NEW\_SERIES\_NAME t\_outflow

LABEL interflow

NEW\_SERIES\_NAME interflow

DATE\_1 6/1/1976

TIME\_1 00:12:00

DATE\_2 7/1/1976

TIME\_2 00:12:00

END GET\_SERIES\_PLOTGEN

DATE\_ and TIME\_ specifiers are optional in a GET\_SERIES\_PLOTGEN block. If they are absent from the block, then the entire time series pertaining to each nominated label is imported. If a DATE\_1 keyword is present but a TIME\_1 keyword is absent, then TIME\_1 is assumed to be 00:00:00; the same applies for DATE\_2. However if TIME\_1 is present then DATE\_1 must also be present; the same holds for TIME\_2.

## GET\_SERIES\_SSF

Instructions provided in a GET\_SERIES\_SSF block allow TSPROC to import a time series from a site sample file; see Appendix B for the format of this file. Because a site sample file is used for time series storage by other members of the PEST Surface Water Utilities suite, TSPROC can readily import time series data written by other members of the suite. Also, if it is desired that TSPROC be used in the calibration of a model for which it is presently incapable of directly importing results, then this can be implemented by writing a small translation program which converts the outputs of that model to site sample file format. This program would be run between the model and TSPROC as part of a composite model calibrated by PEST.

The table below shows the keywords pertaining to a GET\_SERIES\_SSF block. An example of a GET\_SERIES\_SSF block is shown following that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a GET\_SERIES\_SSF block.
2. Example usage of a GET\_SERIES\_SSF block.

START GET\_SERIES\_SSF

CONTEXT all

FILE flows.smp

SITE rebec\_ck

NEW\_SERIES\_NAME rebecca

DATE\_1 06/03/1970

TIME\_1 12:00:00

DATE\_2 09/01/1980

TIME\_1 00:00:00

END GET\_SERIES\_SSF

The DATE\_ and TIME\_ specifiers are optional. If they are omitted then the entire time series pertaining to the nominated site is imported. If a DATE\_1 keyword is present but a TIME\_1 keyword is absent, then TIME\_1 is assumed to be 00:00:00; similarly for DATE\_2. If TIME\_1 is present then DATE\_1 must be present; the same holds for TIME\_2.

## GET\_SERIES\_WDM

Instructions provided in this block allow TSPROC to import a time series from a Watershed Data Management (WDM) file. Many hydrologic and water-quality models and analyses developed by the U.S. Geological Survey and the U.S. Environmental Protection Agency currently use a WDM file. The WDM file is a binary file which provides the user with a common data base for many applications, thus eliminating the need to reformat data from one application to another.

The table below shows the keywords permissible in a GET\_SERIES\_WDM block. An example of a GET\_SERIES\_WDM block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a GET\_SERIES\_WDM block.
2. Example usage of a GET\_SERIES\_WDM block.

START GET\_SERIES\_WDM

CONTEXT all

FILE catchment.wdm

DSN 1013

NEW\_SERIES\_NAME coal\_ck

DATE\_1 06/03/1970

TIME\_1 12:00:00

DATE\_2 09/01/1980

TIME\_1 00:00:00

DEF\_TIME 12:00:00

FILTER –999.99

END GET\_SERIES\_WDM

The DATE\_ and TIME\_ specifiers are optional in a GET\_SERIES\_WDM block. If they are omitted then the entire time series pertaining to the nominated data set number is imported. If a DATE\_1 keyword is present but a TIME\_1 keyword is absent, then TIME\_1 is assumed to be 00:00:00; similarly for DATE\_2. If TIME\_1 is present then DATE\_1 must be present; the same holds for TIME\_2.

If the sample interval for a time series stored in a WDM file is a day or greater, then each term of the series will have no time reference; however within TSPROC each time series term is associated with both a date and a time. When importing such a time series into TSPROC, TSPROC’s default behaviour is to assign each term a time of 00:00:00 on the day with which it is associated. However, this time can be altered to the user’s choice using the optional DEF\_TIME keyword. Note that if DEF\_TIME is supplied as "24:00:00" then each sample will be assigned a time of 00:00:00 on the following day.

## HYDRO\_EVENTS

Using the HYDRO\_EVENTS block, storm hydrographs can be extracted for specific periods within a time series. Optionally, the terms of the series upon which events are extracted can be limited to those events occurring within a specified date/time interval. Another option provided by the HYDRO\_EVENTS block is for events to be extracted using a minimum number of days between peaks and specifying a minimum peak value.

TSPROC stores the outcomes of storm events extracted by the HYDRO\_EVENTS block in a new time series. Like other TSPROC entities, the new time series must be provided with a name so that it can be referenced by other TSPROC processing blocks. This name must be 10 characters or less in length and must not include a space character.

Keywords featured in the HYDRO\_EVENTS block are listed in the following table. An example of a HYDRO\_EVENTS block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a HYDRO\_EVENTS block.
2. Example usage of a HYDRO\_EVENTS block.

START HYDRO\_EVENTS

CONTEXT all

SERIES\_NAME outflow

NEW\_SERIES\_NAME outflow\_pk

WINDOW 7

MIN\_PEAK 10.5

RISE\_LAG 2

FALL\_LAG 6

DATE\_1 10/1/1976

TIME\_1 00:00:00

DATE\_2 9/30/1985

TIME\_2 00:00:00

END HYDRO\_EVENTS

## HYDROLOGIC\_INDICES

Hydrologic indices are statistical measures applied to streamflow records in a way that attempts to quantify various ecologically important aspects of a flow regime. Classes of hydrologic indices include measures that quantify such things as the timing and seasonal pattern of extreme flows, daily, seasonal, and annual flow variability, as well as rates of flow increases and decreases. Over 160 different hydrologic indices may be calculated by means of a HYDROLOGIC\_INDICES block. Computation of the indices is accomplished by means of code adapted from the USGS Hydrologic Index Tool (Henricksen and others, 2006). Because many of the hydrologic indices that can be calculated are somewhat redundant, the user may elect to calculate a subset of the available indices on the basis of the stream’s hydrologic regime type (for example, snowmelt-dominated, groundwater-dominated, surface runoff-dominated). Olden and Poff identified a list of the high-information, non-redundant indices for six hydrologic regime types.

1. Keywords in a HYDROLOGIC\_INDICES block.

Because many of the hydrologic indices that can be calculated are somewhat redundant, the user may elect to calculate a subset of the available indices on the basis of the stream’s hydrologic regime type (for example, snowmelt-dominated, groundwater-dominated, surface runoff-dominated). Olden and Poff (2003) identified a list of the high-information, non-redundant indices for six hydrologic regime types. Table 13 summarizes the arguments that may be supplied to the HYDROLOGIC\_REGIME and FLOW\_COMPONENT keywords in order to generate a subset of hydrologic indices appropriate to the system under study.

1. List of available hydrologic indices and associated arguments.
2. Example usage of a HYDROLOGIC\_INDICES block.

START HYDROLOGIC\_INDICES

CONTEXT all

SERIES\_NAME outflow

NEW\_TABLE\_NAME outflow\_hi

HYDROLOGIC\_REGIME groundwater\_perennial

FLOW\_COMPONENT all

DATE\_1 01/01/1980

TIME\_1 00:00:00

DATE\_2 12/31/1989

TIME\_2 23:59:59

END HYDROLOGIC\_INDICES

## LIST\_OUTPUT

The LIST\_OUTPUT block provides the means whereby the outcomes of calculations carried out by TSPROC can be written to an ASCII (ie. text) file. The format of this file is such that these quantities can be easily read by a user. They can also be easily read by PEST. An instruction file by which PEST can read the contents of a LIST\_OUTPUT file can be generated automatically using the WRITE\_PEST\_FILES block.

Keywords associated with a LIST\_OUTPUT block are recorded in the following table. An example of a LIST\_OUTPUT block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a LIST\_OUTPUT block.
2. Example usage of a GET\_SERIES\_WDM block.

START LIST\_OUTPUT

CONTEXT all

FILE output.txt

SERIES\_NAME flow\_216

SERIES\_NAME flow\_342

V\_TABLE\_NAME vol\_216

V\_TABLE\_NAME vol\_342

S\_TABLE\_NAME st\_216

S\_TABLE\_NAME st\_342

E\_TABLE\_NAME dur\_216

E\_TABLE\_NAME dur\_342

C\_TABLE\_NAME comp\_ser

SERIES\_FORMAT short

END LIST\_OUTPUT

Any number of time series, c\_tables, s\_tables, v\_tables and e\_tables can be written to a file generated by the LIST\_OUTPUT block. Hence as many of the keywords pertaining to these entities as desired can be supplied in this block. In generating its output files, time series are written first, followed by s\_tables, followed by c\_tables, followed by v\_tables, and finally e\_tables. However the ordering of the individual entities of each type within the different segments of the TSPROC output file is the same as the order in which respective keywords referencing those entities are supplied in the LIST\_OUTPUT block.

If a SERIES\_NAME keyword is provided in a LIST\_OUTPUT block then a SERIES\_FORMAT keyword must also be provided; options are "short" and "long". If the former option is supplied, the LIST\_OUTPUT block will list the terms of the time series as a single column in its output file. If the latter option is supplied the terms of the time series will be accompanied by the date and time corresponding to the term, as well as the name of the time series. This format corresponds to that of a site sample file (see Appendix B) and can thus be used by other members of the PEST Surface Water Utilities; note however that the header to each time series, written by the LIST\_OUTPUT block to its output file, must first be removed.

If you are running TSPROC as part of a composite model under the control of PEST, it is best to use the "short" option for time series formatting. This is because, where a time series is large, a considerable amount of computation time may be spent in converting TSPROC’s internal representation of sample dates and times to the dd/mm/yyyy (or mm/dd/yyyy) and hh:mm:ss formats required for output listing. This can add considerably to overall composite model execution time. Note also that if the "long" protocol is employed, in accordance with site sample file protocol, TSPROC does not represent midnight as "24:00:00"; instead midnight is represented as 00:00:00 on the following day.

Output formatting for other TSPROC entities is such that they are clearly labelled and easily understood by the user. In the case of s\_tables and c\_tables, it is important to note that statistics not requested in the SERIES\_STATISTICS or SERIES\_COMPARE block in which an s\_table or c\_table respectively is created are not recorded in the file written by the LIST\_OUTPUT block. Thus if this file is considered as the output file of a composite model, and that composite model is being calibrated by PEST, such statistics will not be included in the calibration process.

Exceedence times stored in an e\_table are recorded by the LIST\_OUTPUT block both as accumulated times, and as proportions of the total time spanned by the parent time series. Note that if this file is used by PEST, only the latter quantities (ie. the exceedence proportions) are actually read by PEST on the basis of the instruction file created through a WRITE\_PEST\_FILES block.

## NEW\_SERIES\_UNIFORM

The NEW\_SERIES\_UNIFORM block creates a uniform-valued time series with series entries placed at uniform (or almost uniform) time intervals. Keywords belonging to the NEW\_SERIES\_UNIFORM block are listed in the following table. An example NEW\_SERIES\_UNIFORM block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a NEW\_SERIES\_UNIFORM block.
2. Example usage of a NEW\_SERIES\_UNIFORM block

START NEW\_SERIES\_UNIFORM

CONTEXT all

TIME\_INTERVAL 2

TIME\_UNIT days

DATE\_1 1/1/2000

TIME\_1 12:00:00

DATE\_2 15/12/2005

TIME\_2 13:00:00

NEW\_SERIES\_NAME series1

NEW\_SERIES\_VALUE 5.0

END NEW\_SERIES\_UNIFORM

The behaviour of the NEW\_SERIES\_UNIFORM block is slightly different depending on whether TIME\_UNIT is supplied as "seconds", "minutes", "hours" or "days" on the one hand, or "months" or "years" on the other hand. In the former case the series time interval is strictly TIME\_INTERVAL times the TIME\_UNIT; thus the time increment between successive terms of the series is strictly uniform. For example, if the TIME\_INTERVAL is supplied as 2 and the TIME\_UNIT is supplied as "hours", then all samples are 2 hours apart. The first sample occurs on DATE\_1, TIME\_1; the last sample is no later than DATE\_2, TIME\_2. (Note that, in contrast to most other blocks, all of the DATE\_1, TIME\_1, DATE\_2 and TIME\_2 keywords must be supplied.)

On the other hand if TIME\_UNIT is set to "months", then all terms of the new series occur on the same day of the month, and at the same time as the initial time TIME\_1. Thus terms are variously 28, 29, 30 or 31 days apart. (In this case TSPROC will reject a DATE\_1 in which the date is 29th, 30th or 31st of the month.) If TIME\_UNIT is set to "years", then all terms of the new time series occur on the same date, but separated by TIME\_INTERVAL years. In this case TSPROC will not allow DATE\_1 to be 29th February.

All terms of the new series are assigned the same value, this being the user-supplied NEW\_SERIES\_VALUE.

The NEW\_TIME\_SERIES block can be useful as a precursor to digital filtering. As explained in documentation to the DIGITAL\_FILTER block, digital filtering can only take place on a time series for which the terms are separated by a constant time increment. If filtering must be performed on an observed time series that has not been sampled at such a constant increment, the latter can be interpolated to a constant time base series (created using the NEW\_SERIES\_UNIFORM block) using the NEW\_TIME\_BASE block. Filtering can then be undertaken on the interpolated time series.

## NEW\_TIME\_BASE

The NEW\_TIME\_BASE block is used to carry out time-interpolation from the sample times pertaining to one time series to the sample times pertaining to another. Keywords belonging to the NEW\_TIME\_BASE block are listed in the following table. An example NEW\_TIME\_BASE block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a NEW\_TIME\_BASE block.
2. Example usage of a NEW\_TIME\_BASE block.

START NEW\_TIME\_BASE

CONTEXT all

SERIES\_NAME mod\_flow

TB\_SERIES\_NAME obs\_flow

NEW\_SERIES\_NAME int\_flow

END NEW\_TIME\_BASE

Time interpolation of one time series to the time-base of another will only occur if the time-span of the latter time series is equal to, or smaller than, that of the former time series. The result will be a new time series with terms pertaining to exactly the same dates and times as those of the time-base time series. If the original time series and the time-base time series pertain to the same data type, this will allow the two series to be directly compared with each other. Such a comparison of "apples with apples" is crucial when calibrating a model against field data. Hence one of the principal roles of TSPROC when used as a model post-processor in a "composite model" run by PEST, is to carry out this all-important time-interpolation of model-generated time series to the dates and times of their measured counterparts. An interpolated time series produced in this manner can then be written to a TSPROC output file (using the LIST-OUTPUT block), where it can be read by PEST and compared with measured values recorded in a PEST control file. Both the PEST control file, and the instruction file by which the time-interpolated time series can be read from the LIST\_OUTPUT file, can be written using the WRITE\_PEST\_FILES block.

## PERIOD\_STATISTICS

Using the PERIOD\_STATISTICS block, a number of simple statistics can be calculated for specific periods within a time series. Optionally, the terms of the series upon which statistical calculations are based can be limited to those lying within a specified date/time interval. Another option provided by the PERIOD\_STATISTICS block is for statistics to be calculated on the basis of the log (to base 10) of the terms of the time series, or on the terms of the series raised to an arbitrary power. If it is desired that statistics be calculated on the basis of more complex functions of the terms of a time series, this can be easily achieved by first calculating a new time series using the SERIES\_EQUATION block, and then undertaking statistical calculations on the basis of this new time series.

At present, only 6 statistical measures can be calculated using the PERIOD\_STATISTICS block. These are the mean, standard deviation, sum, maximum, minimum and range. In addition, the supported periods are monthly and yearly (calendar year or water year).TSPROC stores the outcomes of statistical calculations carried out by the PERIOD\_STATISTICS block in a new time series. Like other TSPROC entities, the new time series must be provided with a name so that it can be referenced by other TSPROC processing blocks. This name must be 10 characters or less in length and must not include a space character.

Keywords featured in the PERIOD\_STATISTICS block are listed in the following table. An example of a PERIOD\_STATISTICS block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a PERIOD\_STATISTICS block.
2. Example usage of a PERIOD\_STATISTICS block.

START PERIOD\_STATISTICS

CONTEXT all

SERIES\_NAME outflow

NEW\_SERIES\_NAME outflow\_m

STATISTIC mean

PERIOD month\_many

TIME\_ABSCISSA start

LOG yes

DATE\_1 10/1/1976

TIME\_1 00:00:00

DATE\_2 9/30/1985

TIME\_2 00:00:00

END PERIOD\_STATISTICS

Caution should be exercised when using the POWER and LOG keywords. It is illegal for both of these keywords to be present within the same SERIES\_STATISTICS block. Furthermore, there is a potential for numerical errors to occur through the use of these keywords. In particular if LOG is set to “yes” and if any of the terms of the time series are zero or negative, TSPROC will cease execution with an appropriate error message. Also if a POWER with an absolute value of less than 1 is supplied and if any of the terms of the time series are negative, or if the POWER is negative and any of the terms of the time series are zero, TSPROC will likewise cease execution with an error message before attempting this impossible calculation.

The high-flow water year begins October 1 of the previous year and ends September 30 of an individual year. The low-flow water year begins April 1 of the previous year and ends March 31 of an individual year. The calendar year begins January 1 and ends December 31 of an individual year.

For monthly statistics, selecting “period\_many” as the PERIOD keyword will compute a monthly statistic for each year in the input time series. Alternatively, selecting “period\_one” as the PERIOD keyword will compute a single statistic for each month, aggregating across all years in the input time series. When computing a mean, the “period\_many” mean is commonly called the monthly mean value, whereas the “period\_one” mean is commonly called the mean monthly value.

## REDUCE\_TIME\_SPAN

The REDUCE\_TIME\_SPAN block reduces the time spanned by a time series. This may be a useful precursor to other aspects of TSPROC processing. For example, using the REDUCE\_TIME\_SPAN block, the time spanned by an "observed time series" can be reduced to that spanned by a model-generated time series. This will allow time interpolation from the model’s output times to the times at which measurements were made, to be carried out using the NEW\_TIME\_BASE block.

Keywords found in a REDUCE\_TIME\_SPAN block are listed in the table below. An example of a REDUCE\_TIME\_SPAN block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a REDUCE\_TIME\_SPAN block.
2. Example usage of a REDUCE\_TIME\_SPAN block.

START REDUCE\_TIME\_SPAN

CONTEXT all

SERIES\_NAME intflow

NEW\_SERIES\_NAME intflow\_1

DATE\_1 02/01/1976

TIME\_1 13:13:00

DATE\_2 06/01/1976

TIME\_2 00:00:00

END REDUCE\_TIME\_SPAN

When a new time series is created by reducing the time span of an existing time series, the original time series still remains within TSPROC’s memory. If desired, it can be removed using the ERASE\_ENTITY block.

At least one of DATE\_1 or DATE\_2 must be supplied. If the corresponding TIME\_ keyword is not supplied, a default time of 00:00:00 is used. If the DATE\_1 keyword is omitted DATE\_1 and TIME\_1 are assumed to be the first date and time cited in the original time series, ie. no time-span reduction from the front of the time series takes place. Similarly, if the DATE\_2 keyword is omitted, no time-span reduction takes place from the end of the existing time series. Note that a TIME\_ keyword cannot be supplied without the corresponding DATE\_ keyword.

## SERIES\_BASE\_LEVEL

Use of the SERIES\_BASE\_LEVEL block allows a user to subtract a constant amount from all terms of a time series. This constant amount is the value of one term of an existing time series, either the time series from which subtraction is taking place, or another time series stored within the memory of TSPROC.

A common use of the SERIES\_BASE\_LEVEL block is in calculation of changes in the quantity represented by the time series over the data recording or model simulation interval that gave rise to the time series in the first place. In this case the first term of the time series may be taken as the base level, this term being subtracted from all other elements of the time series to create the new series with altered base level. SERIES\_BASE\_LEVEL functionality allows this new series to either replace the original time series or to exist as its own separate entity.

Keywords found in a SERIES\_BASE\_LEVEL block are listed in the table below. An example of a SERIES\_BASE\_LEVEL block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a SERIES\_BASE\_LEVEL block.
2. Example usage of a SERIES\_BASE\_LEVEL block.

As is documented elsewhere in this manual, the SERIES\_EQUATION block can also be used to subtract a constant from the terms of a series. However in that case, the constant is supplied as a number in an equation. In the case of the SERIES\_BASE\_LEVEL block, the subtractor is a term in a series, identified through the name of the series and the date and time to which the term pertains. If there is no term corresponding to the supplied date and time, TSPROC will cease execution with an appropriate error message.

The NEGATE keyword can be useful in incidences such as where it is desired that drawdown be calculated from head. Drawdown is calculated as the negative of the change in head from its initial value. Thus after base level alteration by subtraction of the initial series term, all terms of the new time series are multiplied by –1.

## SERIES\_CLEAN

Using the SERIES\_CLEAN block, unwanted terms can be eliminated from a time series or replaced with a preferred value. This is sometimes required for correcting the deleterious effects of model misbehaviour whereby model-generated time-series are "polluted" with intermittent spurious values. It can also be used for eliminating outliers in an observation time series.

Keywords pertaining to the SERIES\_CLEAN block are listed in the table below. An example SERIES\_CLEAN block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a SERIES\_CLEAN block.
2. Example usage of a SERIES\_CLEAN block.

START SERIES\_CLEAN

CONTEXT all

SERIES\_NAME series1

LOWER\_ERASE\_BOUNDARY 100.0

UPPER\_ERASE\_BOUNDARY 200.0

SUBSTITUTE\_VALUE delete

NEW\_SERIES\_NAME series2

END SERIES\_CLEAN

The SERIES\_CLEAN block presents the user with a number of different options for handling unwanted terms. In the simplest case these terms are replaced by the number supplied through the SUBSTITUTE\_VALUE keyword. If this is done, terms can be replaced "in situ" (ie. in the existing time series without creating a new one), or a new time series can be created to hold the altered time series, with the original time series remaining intact. If a NEW\_SERIES\_NAME keyword is supplied, the latter option is taken; if not, the former option is taken.

A further option is for unwanted terms to be eradicated altogether. This is achieved by supplying the string "delete" with the SUBSTITUTE\_VALUE keyword instead of a real number. In this case TSPROC insists that a NEW\_SERIES\_NAME keyword be supplied in the SERIES\_CLEAN block, for the altered time series will be stored as a new entity, leaving the original one intact; the latter can then be erased if desired using the ERASE\_ENTITY block.

Terms of a series are identified for deletion or replacement using the LOWER\_ERASE\_BOUNDARY and UPPER\_ERASE\_BOUNDARY keywords. Either one or both of these keywords can be supplied. If both of them are supplied, all terms of the time series between and including the specified boundary values are replaced or deleted. If only the LOWER\_ERASE\_BOUNDARY keyword is supplied, all terms equal to and above this threshold are removed or replaced; if only the UPPER\_ERASE\_BOUNDARY keyword is supplied, all terms equal to or below this boundary are removed or replaced. (If you are in any doubt of the action of the SERIES\_CLEAN block when only one of these keywords is supplied, then supply both of them, with one of them either very high or very low. However if you do this, note that TSPROC will not accept numbers whose absolute value is greater than about 1.0E+37.

## SERIES\_COMPARE

The SERIES\_COMPARE block calculates statistics that quantify the similarity of one time series with another. The outcomes of these calculations are placed in a c\_table (which can be written to a file using the LIST\_OUTPUT block). Keywords pertaining to the SERIES\_COMPARE block are listed in the table below. An example SERIES\_COMPARE block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a SERIES\_COMPARE block.
2. Example usage of a SERIES\_COMPARE block.

START SERIES\_COMPARE

CONTEXT all

SERIES\_NAME\_SIM mod\_flow

SERIES\_NAME\_OBS obs\_flow

NEW\_C\_TABLE\_NAME com\_series

BIAS yes

RELATIVE\_BIAS yes

STANDARD\_ERROR yes

RELATIVE\_STANDARD\_ERROR yes

NASH\_SUTCLIFFE yes

COEFFICIENT\_OF\_EFFICIENCY yes

INDEX\_OF\_AGREEMENT yes

EXPONENT 1

END SERIES\_COMPARE

The names of two time series must be provided in a SERIES\_COMPARE block. One of these is denoted as the "observed" time series while the other is the "simulated" time series; the difference is important in calculating relative bias, relative standard error, the Nash-Sutcliffe coefficient , the index of agreement and the coefficient of efficiency, for standardisation of these quantities is undertaken with respect to the observed time series. The simulated and observed time series must contain samples taken at identical dates and times within the time interval spanned by the DATE\_1, TIME\_1 and DATE\_2, TIME\_2 entries. If these keywords are not provided the sample dates and times of the observed and simulated time series must be identical over the entire length of these series.

If either of the COEFFICIENT\_OF\_EFFICIENCY or INDEX\_OF\_AGREEMENT keywords are present, then an EXPONENT keyword must be present. The theory underpinning use of the coefficient of efficiency and index of agreement as bases for series comparison is discussed in Legates and McCabe . The exponent must be either 1 or 2. If either of these keywords are present, then a SERIES\_NAME\_BASE keyword can also be supplied, this providing the name of a "baseline time series" that can optionally be used in place of the mean observation value over the comparison time window; see the above reference for details. The baseline time series must have terms at identical dates and times to those of the simulated and observed time series over the comparison time window. If the SERIES\_NAME\_BASE keyword is omitted, then the mean observation is employed in the formulae presented below instead of the terms of the baseline time series.

Equations for the quantities calculated in the SERIES\_COMPARE block are as follows. Note that the Nash-Sutcliffe coefficient is equal to the coefficient of efficiency when the exponent in the latter equation is zero, and when a baseline time series is not provided.

Bias:

 (1)

Standard error:

 (2)

Relative bias:

 (3)

Relative standard error:

 (4)

Nash-Sutcliffe coefficient:

 (5)

Coefficient of efficiency:

` (6)

*Index of agreement:*

 (7)

where:

 (8)

and N is the number of terms in the series (or subseries) between which comparison takes place; summation in the above equations takes place over all of these terms. Where a SERIES\_NAME\_BASE keyword is supplied, in the equations for coefficient of efficiency and index of agreement is replace by Bi, the respective term of the baseline time series.

If it is desired that weights be applied to terms of the series before comparison (as is often the case), weighted observation and simulated time series can easily be generated using the SERIES\_EQUATION block.

## SERIES\_DIFFERENCE

The SERIES\_DIFFERENCE block is used to calculate a new time series, the terms of which are differences between successive terms of an existing time series. Keywords pertaining to the SERIES\_DIFFERENCE block are listed in the table below. An example SERIES\_DIFFERENCE block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a SERIES\_DIFFERENCE block.
2. Example usage of a SERIES\_DIFFERENCE block.

A SERIES\_DIFFERENCE block.

START SERIES\_DIFFERENCE

CONTEXT all

SERIES\_NAME 322

NEW\_SERIES\_NAME 322\_d

END SERIES\_DIFFERENCE

The outcome of processing a SERIES\_DIFFERENCE block is another time series, the terms of which are the differences between successive terms of an existing time series. Where successive terms are subtracted in this manner, the difference is ascribed to the date and time pertaining to the later of the two terms. The new time series therefore has one less term than the original time series, for no term exists in the new time series with the same date and time as that of the first term in the existing time series.

## SERIES\_DISPLACE

The SERIES\_DISPLACE block is used to "migrate" the terms of a series with respect to its time-base, lagging or leading these terms as requested by the user. Keywords pertaining to the SERIES\_DISPLACE block are listed in the table below. An example SERIES\_DISPLACE block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a SERIES\_DISPLACE block.
2. Example usage of a SERIES\_DIFFERENCE block.

START SERIES\_DISPLACE

CONTEXT all

SERIES\_NAME outflow

NEW\_SERIES\_NAME outflow\_1

LAG\_INCREMENT 1

FILL\_VALUE 0.00

END SERIES\_DISPLACE

The SERIES\_DISPLACE operation is the only procedure undertaken by TSPROC which requires that the time series upon which the operation is carried out have a constant sample interval. If the sample interval is not constant throughout the time spanned by the time series, TSPROC will display an appropriate error message before ceasing execution.

A positive LAG\_INCREMENT is used to delay terms in the time series. For example, if a LAG\_INCREMENT of 1 is used, then each term within a time series will be assigned to the time and date previously occupied by the term which follows it. If it is desired that terms in the series be shifted in the opposite direction instead, this can be accomplished by using a negative LAG\_INCREMENT.

When terms of a time series are shifted in this manner, terms at one end of the series "drop off the edge" (the time-base of the series is not altered by the SERIES\_DISPLACE operation). At the other end of the series, at least one term of the shifted series must be assigned a "dummy value" as end positions within the series become vacated by the shifting operation. The user must provide this "dummy value" using the FILL\_VALUE keyword.

In undertaking sophisticated (and extremely powerful) parameter estimation procedures such as that described by Kuczera (1983), it is necessary that a combination of an original and a lagged "observed time series" be compared with its model-generated counterpart. Residuals (ie. model-to-measurement differences) achieved through the model calibration process using such combinations of time series are often superior to those achieved using the original time series because the former have drastically reduced inbuilt inter-term correlation structure. The existence of such inter-term correlation can lead to misleading estimates of parameter uncertainty.

A composite series, comprised of an original time series summed with various combinations of lagged time series, can be created using the SERIES\_EQUATION block.

## SERIES\_EQUATION

Through use of the SERIES\_EQUATION block a new time series can be formed based on an equation of arbitrary mathematical complexity involving one or a number of other time series. The only two conditions on time series that are cited in this equation are that:-

1. all time series featured in the series equation must have samples at identical dates and times (this can be ensured by using the REDUCE\_TIME\_SPAN and NEW\_TIME\_BASE blocks if necessary), and

2. a series equation must feature at least one time series (in order to provide the time-base of the resulting time series).

Keywords appearing in a SERIES\_EQUATION block are listed in the following table. An example of a SERIES\_EQUATION block follows the table. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a SERIES\_EQUATION block.
2. Example usage of a SERIES\_DIFFERENCE block.

START SERIES\_EQUATION

CONTEXT all

NEW\_SERIES\_NAME new\_series

EQUATION log10(outflow \* concentration)

END SERIES\_EQUATION

The terms of the new time series that results from the action of the series equation are computed by implementing the equation on a term-by-term basis on each of the series cited in the equation. Thus each term in the new series is calculated from the corresponding terms of the existing series.

As stated above, the series equation can be of arbitrary complexity, involving any number of terms, and citing any number of existing time series (as long as the above-mentioned time-base-consistency rule is followed). In formulating the equation, the operators "^", "/", "\*", "-" and "+" have their usual meanings of "raised to the power of", "division", "multiplication", "subtraction" and "addition"; optionally the "\*\*" operator can be used in place of the "^" operator to signify raising to the power. Operations are carried out in the order indicated above (ie. the normal ordering of mathematical operations); if in doubt, use brackets to set precedence between operators.

An equation supplied in the SERIES\_EQUATION block can include most of the commonly-used mathematical functions, viz. abs, acos, asin, atan, cos, cosh, exp, log, log10, sin, sinh, sqrt, tan and tanh. Note the following:-

1. The log function is to base e; to calculate logs to base 10, use the log10 function.
2. The arguments to trigonometric functions must be supplied in radians.
3. Caution must be exercised when using some of these functions that their argument lies within the proper numerical range for that function. For example, if any of the terms of a series upon which a log operation is performed are zero or negative, a numerical error will result. TSPROC will detect this error and cease execution with an appropriate error message.

Caution must also be exercised when using the "/" operator that a divide-by-zero condition is not encountered. If this occurs, TSPROC will issue an appropriate error message before ceasing execution.

In addition to the above functions, TSPROC allows two "native TSPROC functions" to be used in a series equation; these are the @\_days\_start\_year and @\_days\_"mm/dd/yyyy\_hh:nn:ss" functions (the "@\_" string indicates to the subroutine that parses this equation that the term represents neither a series, a number, nor one of the mathematical functions discussed above).

When the @\_days\_start\_year term is encountered in a series equation, the days since the start of the year pertaining to the current series term is substituted for the string. Where a sample does not occur at midnight, fractional days are used in the calculation of the @\_days\_start\_year function, the outcome of which is a real number.

When the @\_days\_"mm/dd/yyyy\_hh:nn:ss" term is encountered, TSPROC calculates the days (as a real number – fractional if necessary) since the indicated date and time. Note that the date and time strings must be collectively enclosed in quotes and must be separated by an underscore. Note also that the correct format to use in expressing the date (ie. mm/dd/yyyy or dd/mm/yyyy) is determined by the DATE\_FORMAT keyword in the SETTINGS block.

The following are some examples of legal series equations.

1. Examples of legal EQUATION arguments.

outflow

log10(outflow) + 3.456 \* sediment ^ 3.23

34.5 / (interflow + 3.432)

0.0 \* series1 + @\_days\_start\_year

3.495 + sin((@\_days\_start\_year + 124.5)\*6.284/365.25)

1.0/sqrt(@\_days\_"1/21/1978\_12:00:00")

In the third of the above equations the time series named series1 is multiplied by zero. In this case the series is included in the equation because of the fact that each equation must cite at least one time series in order to set the time-base of the resultant time series. In the fourth of the above equations the argument of the sine function is multiplied by  in order to achieve periodicity of one year.

Note that, for those not familiar with programming, the equation a/b\*c is evaluated as (a/b)\*c. To divide a by b\*c formulate the equation as: a/(b\*c) or a/b/c.

## SERIES\_STATISTICS

Using the SERIES\_STATISTICS block, a number of simple statistics can be calculated from the terms of a time series. Optionally, the terms of the series upon which statistical calculations are based can be limited to those lying within a specified date/time interval. Another option provided by the SERIES\_STATISTICS block is for statistics to be calculated on the basis of the log (to base 10) of the terms of the time series, or on the terms of the series raised to an arbitrary power. If it is desired that statistics be calculated on the basis of more complex functions of the terms of a time series, this can be easily achieved by first calculating a new time series using the SERIES\_EQUATION block, and then undertaking statistical calculations on the basis of this new time series.

At present, only 8 statistical measures can be calculated using the SERIES\_STATISTICS block. These are the mean, standard deviation, sum, maximum, minimum, range the minimum n point mean and the maximum n point mean. Note that, as is explained below, if it is intended to use any statistics in a calibration exercise undertaken by PEST, then only those statistics that are actually involved in the parameter estimation process should be calculated in a SERIES\_STATISTICS block. This, in turn, will limit the output from the LIST\_OUTPUT block to only those statistics.

TSPROC stores the outcomes of statistical calculations carried out by the SERIES\_STATISTICS block in an s\_table. Like other TSPROC entities, each s\_table must be provided with a name so that it can be referenced by other TSPROC processing blocks. This name must be 10 characters or less in length and must not include a space character.

Keywords featured in the SERIES\_STATISTICS block are listed in the following table. An example of a SERIES\_STATISTICS block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a SERIES\_STATISTICS block.
2. Example usage of a SERIES\_DIFFERENCE block.

START SERIES\_STATISTICS

CONTEXT all

SERIES\_NAME outflow

NEW\_S\_TABLE\_NAME outflow

MEAN yes

STANDARD\_DEVIATION yes

SUM yes

MAXIMUM yes

MINIMUM yes

MINMEAN\_5 yes

MAXMEAN\_5 yes

POWER 0.5

DATE\_1 3/1/1976

TIME\_1 00:00:00

DATE\_2 3/3/1976

TIME\_2 00:00:00

END SERIES\_STATISTICS

Caution should be exercised when using the POWER and LOG keywords. It is illegal for both of these keywords to be present within the same SERIES\_STATISTICS block. Furthermore, there is a potential for numerical errors to occur through the use of these keywords. In particular if LOG is set to "yes" and if any of the terms of the time series are zero or negative, TSPROC will cease execution with an appropriate error message. Also if a POWER with an absolute value of less than 1 is supplied and if any of the terms of the time series are negative, or if the POWER is negative and any of the terms of the time series are zero, TSPROC will likewise cease execution with an error message before attempting this impossible calculation.

The MINMEAN\_n and MAXMEAN\_n statistics require further explanation. As is apparent from the above example, the user must supply an appropriate value for n him/herself. Thus, for example, if MINMEAN\_5 is set to "yes", TSPROC calculates the minimum value of the running mean of 5 consecutive values of the series, this calculation taking place over the length of the series, or between the user-provided beginning and end dates. It is important to note that if both the MINMEAN\_n and MAXMEAN\_n keywords are supplied in the same SERIES\_STATISTICS block, n must be the same for both of these keywords. Note also, that the LOG and POWER keywords must not be supplied in the same block as the MINMEAN\_n and MAXMEAN\_n keywords; if this is a problem, use the SERIES\_EQUATION block to transform the series prior to use of the SERIES\_STATISTICS block.

## SETTINGS

The SETTINGS block differs from the other blocks in a TSPROC input file in that it must be the first block listed in this file; furthermore its presence is mandatory.

At the present stage of TSPROC development, only two keywords can be used in a SETTINGS block; both of these are mandatory. See the table below.

1. Keywords within a SETTINGS block.
2. Example usage of a SETTINGS block.

START SETTINGS

DATE\_FORMAT mm/dd/yyyy

CONTEXT pest\_input

END SETTINGS

The DATE\_FORMAT setting allows TSPROC to adapt to the different methods by which the date is represented in different countries. If the month precedes the day, then the date format should be supplied as "mm/dd/yyyy". However if the day precedes the month, then it should be written as "dd/mm/yyyy".

A SETTINGS block can contain only one CONTEXT keyword, the purpose of this being to "set the context" of the entire TSPROC run. Every other block used in a TSPROC input file must contain a minimum of one, and a maximum of five, CONTEXT keywords followed by a character string (of 20 characters or less in length and without internal spaces). If any of these character strings match the CONTEXT character string provided in the SETTINGS block, or if any of these strings is supplied as "all", then that block will be processed.

Use of TSPROC CONTEXT functionality allows the user to vary the tasks carried out by TSPROC by simply varying one entry in its input file, viz. the CONTEXT variable supplied in the SETTINGS block. This can be particularly useful when using TSPROC in conjunction with PEST. In preparing for a PEST run, a user can set up a complex TSPROC input file which processes both measured and model-generated time series, and then generates a PEST input dataset in which the terms of the processed measured time series act as "calibration targets" to which the terms of the processed model-generated time series are matched. If CONTEXT settings in the various TSPROC processing blocks are carefully selected, it will then be possible for the same TSPROC input file to be used by TSPROC in its capacity as a model post-processor, simply by altering the run CONTEXT in the SETTINGS block.

## USGS\_HYSEP

Using the USGS\_HYSEP block, baseflow can be separated from total flow for specific periods within a time series.

TSPROC stores the outcomes of baseflow\_separation by the USGS\_HYSEP block in a new time series. Like other TSPROC entities, the new time series must be provided with a name so that it can be referenced by other TSPROC processing blocks. This name must be 10 characters or less in length and must not include a space character.

Keywords featured in the USGS\_HYSEP block are listed in the following table. An example of a USGS\_HYSEP block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords within a USGS\_HYSEP block.
2. Example usage of a USGS\_HYSEP block.

The techniques used for baseflow separation are described in the following publication: Sloto, R.A., and Crouse, M.Y., 1996, HYSEP: A computer program for streamflow hydrograph separation and analysis: U.S. Geological Survey Water-Resources Investigations Report 96-4040, 46 p.

Each technique uses a time interval to perform the separation, which is usually based on the following formula for time of concentration (time interval following cessation of rainfall where surface runoff occurs):



Where tc is time of concentration in days, and A is drainage area in mi2. In general, the interval used should be twice the width of the time of concentration, rounded to the nearest odd integer. However, any odd integer can be entered for the TIME\_INTERVAL keyword.

## V\_TABLE\_TO\_SERIES

The V\_TABLE\_TO\_SERIES block copies information stored in a v\_table to a new time series. Information stored in time series format has access to more processing functionality than that available for v\_tables, including calculation of comparison statistics with other series, digital filtering, time interpolation etc.

Keywords associated with the V\_TABLE\_TO\_SERIES block are listed in the following table. An example of a V\_TABLE\_TO\_SERIES block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a V\_TABLE\_TO\_SERIES block.
2. Example usage of a SETTINGS block.

START V\_TABLE\_TO\_SERIES

CONTEXT all

V\_TABLE\_NAME volume

NEW\_SERIES\_NAME ssvol

TIME\_ABSCISSA end

END V\_TABLE\_TO\_SERIES

As is apparent when the contents of a v\_table are written to file using the LIST\_OUTPUT block, there are two dates and times associated with every term of a v\_table, ie. the date and time corresponding to the beginning of the interval over which volume was accumulated, and the date and time corresponding to the end of the interval. However there is only one date and time associate with every time series entry. Thus in transferring data between the two entity types, the user must inform TSPROC how time series dates and times are calculated from v\_table dates and times. Three options are available:

1. Time series dates and times can correspond to the beginnings of respective volume accumulation intervals of the v\_table from which they are derived;
2. Time series dates and times can correspond to the ends of respective volume accumulation intervals of the v\_table from which they are derived;
3. Time series dates and times can correspond to the centres of respective volume accumulation intervals of the v\_table from which they are derived.

Selection of the appropriate one of these three options is undertaken by providing the character string "start", "end" or "centre" (or "center") with the TIME\_ABSCISSA keyword of a V\_TABLE\_TO\_SERIES block.

## VOLUME\_CALCULATION

The VOLUME\_CALCULATION block instructs TSPROC to integrate a time series with respect to time over the time-span bracketed by two dates and times. While the most obvious application of this functionality is in volume calculation, it can also be used for mass calculation if the integration is carried out on a time series which represents the mass flux of some constituent. A mass flux time series can be calculated from time series representing concentration and flow using the SERIES\_EQUATION block.

Integration can be carried out over one or multiple time spans. These time spans are defined in a "dates file", the format of which is illustrated below. Dates and times are supplied in a dates file rather than as part of the VOLUME\_CALCULATION block because in many instances of model calibration a large number of volumes or constituent masses may be used in the calibration process. In some circumstances integration may take place over regularly spaced (for example monthly) time intervals, whereas in other cases integration may take place over a number of discrete, significant events.

1. Example of a dates file.

03/12/1976 11:23:53 04/03/1976 03:00:00

04/30/1976 12:43:00 09/02/1976 23:59:59

04/30/1976 12:43:00 04/30/1976 23:59:59

A dates file can be of any length. Each line must contain 4 entries, viz. the date and time defining the beginning of the integration interval and the date and time defining the end of the interval. The date format must be dd/mm/yyyy or mm/dd/yyyy; the option chosen must be consistent with the DATE\_FORMAT setting in the TSPROC SETTINGS block.

The outcomes of TSPROC’s volume calculations are stored in a v\_table. Like other TSPROC entities, each v\_table must be given a name; this name is supplied through the NEW\_V\_TABLE\_NAME keyword. This, and other keywords associated with a VOLUME\_CALCULATION block are listed in the following table. An example of a VOLUME\_CALCULATION block follows that. Keywords can be supplied in any order, except for the CONTEXT keyword(s) which must precede all others.

1. Keywords in a VOLUME\_CALCULATION block.
2. Example usage of a VOLUME\_CALCULATION block.

START VOLUME\_CALCULATION

CONTEXT all

SERIES\_NAME outflow

NEW\_V\_TABLE\_NAME volout

FLOW\_TIME\_UNITS days

DATE\_FILE "volume dates.dat"

FACTOR 3.4953

END VOLUME\_CALCULATION

Two VOLUME\_CALCULATION keywords require further explanation. The first is the TIME\_UNITS keyword; using this keyword, the user must supply the time units employed by the flow time series. For example if flow is recorded in cubic feet per second, then TIME\_UNITS should be provided as "sec". The second is the optional FACTOR keyword. With this keyword the user should supply a multiplier which TSPROC applies to each integrated volume or mass which it calculates. The predominant use of this multiplier is in units conversion. For example if it were desired that the volume in cubic feet calculated in the above example be stored in units of acre feet, gallons, megalitres or some other volumetric unit, then the appropriate conversion factor should be supplied.

## WRITE\_PEST\_FILES

### General

The WRITE\_PEST\_FILES block instructs TSPROC to generate PEST input files for a parameter estimation run. Use of this block to generate PEST input files is predicated on the assumption that TSPROC will be used as a model post-processor as part of a composite model (encapsulated in a batch or script file) run by PEST. It is further assumed that the input file supplied to TSPROC when used in this mode is almost identical to that used by TSPROC to generate the PEST input files upon which the parameter estimation process is based. However when used in the latter capacity, a number of items specific to construction of the PEST input dataset are enabled using TSPROC CONTEXT functionality. These processing options must then be disabled once the PEST input dataset has been written, and before TSPROC assumes its role as a model post-processor.

### Position within a TSPROC Input File

If present, a WRITE\_PEST\_FILES block must immediately follow a LIST\_OUTPUT block in a TSPROC input file. In writing the PEST input dataset, TSPROC assumes that the LIST\_OUTPUT block which immediately precedes the WRITE\_PEST\_FILES block is exactly the same as that which it will use to generate "model output files" when run as a model post-processor in the forthcoming calibration run. The time series, s\_tables, v\_tables and e\_tables which are cited in the LIST\_OUTPUT block are thus classified as the "model" time series, s\_tables, v\_tables and e\_tables. For each of these model-generated entities a corresponding "observation" entity must be supplied. Like the model entities to which they are matched, the observation entities must have been generated (or simply imported) during the current TSPROC run. (Like the WRITE\_PEST\_FILES block itself, some of the functionality implemented by TSPROC to generate observation entities used by the WRITE\_PEST\_FILES block will probably be disabled through appropriate CONTEXT selection before the current TSPROC input file is supplied to TSPROC for use in its forthcoming role as a model post-processor.)

### Model and Observation Entities

It is important to note that any model entity that is matched to an observation entity must have the same design specifications as that entity. Thus an observation time series must have the same number of terms as the model time series to which it is matched, and each of the terms in these paired time series must pertain to the same date and time. This can be achieved using the REDUCE\_TIME\_SPAN and NEW\_TIME\_BASE blocks; using the former block an observation time series can be contracted in length to the time spanned by a model simulation run, while model outputs can be time-interpolated to measurement times using the latter block. Model and observation s\_tables must include the same statistics, calculated over the same time spans; however a model s\_table will normally have been calculated on the basis of a model-generated time series, whereas an observation s\_table will have been calculated on the basis of an observation time series. Similarly, exceedence times contained in model and observation e-tables must have been calculated from model-generated and observation time series using the same flow thresholds; and model and observation v\_tables must have been calculated from model-generated and observation time series using the same set of integration time intervals. Should TSPROC detect any inconsistencies in such paired entities, it will cease execution with an appropriate error message.

It is a very good idea for model s\_tables, v\_tables and e\_tables to be calculated from model-generated time series after the latter have been time-interpolated to the times and dates of the observation time series to which they correspond. This is especially important if observations are intermittent and irregular. By doing this, any bias or miscalculation of the quantities stored within the various TSPROC entities is "cancelled out" in the calibration process because both the model and observation quantities are subject to exactly the same error caused by limitations in the time base on which they were calculated. If desired, exact calculations of these quantities can be made on the basis of model-generated time series after the calibration process is complete.

### Keywords

The following table describes the keywords associated with a WRITE\_PEST\_FILES block.

1. Keywords in a WRITE\_PEST\_FILES block.

An example of a WRITE\_PEST\_FILES block follows. Note that while this example is based on the use of only one time series, s\_table, v\_table and e\_table in the inversion process, others of each of these entities could have been included simply through adding the appropriate sets of keywords and associated entries to the block below.

1. Example of a WRITE\_PEST\_FILES block.

START WRITE\_PEST\_FILES

CONTEXT pest\_input

NEW\_PEST\_CONTROL\_FILE case.pst

AUTOMATIC\_USER\_INTERVENTION yes

TEMPLATE\_FILE catchment.tpl

MODEL\_INPUT\_FILE catchment.uci

NEW\_INSTRUCTION\_FILE observation.ins

OBSERVATION\_SERIES\_NAME flow\_obs

MODEL\_SERIES\_NAME i\_flow\_mod

SERIES\_WEIGHTS\_EQUATION 1.0/@\_abs\_value

SERIES\_WEIGHTS\_MIN\_MAX 1.0 1000.0

OBSERVATION\_V\_TABLE\_NAME vol\_obs

MODEL\_V\_TABLE\_NAME vol\_mod

V\_TABLE\_WEIGHTS\_EQUATION 5.0

OBSERVATION\_S\_TABLE\_NAME stat\_obs

MODEL\_S\_TABLE\_NAME stat\_mod

S\_TABLE\_WEIGHTS\_EQUATION 1.0/@\_abs\_value

OBSERVATION\_E\_TABLE\_NAME time\_obs

MODEL\_E\_TABLE\_NAME time\_mod

E\_TABLE\_WEIGHTS\_EQUATION log(2.0/@\_abs\_value) + 2.0

E\_TABLE\_WEIGHTS\_MIN\_MAX 0 1000

PARAMETER\_DATA\_FILE param.dat

PARAMETER\_GROUP\_FILE pargroup.dat

MODEL\_COMMAND\_LINE model.bat

END WRITE\_PEST\_FILES

### Tasks Undertaken by TSPROC in Generating a PEST Input Dataset

In processing the entries contained within a WRITE\_PEST\_FILES block, TSPROC undertakes the following tasks.

1. It reads all template files cited in the WRITE\_PEST\_FILES block, accumulating the names of all parameters cited in those files.
2. If a PARAMETER\_DATA\_FILE keyword is present within the WRITE\_PEST\_FILES block, TSPROC reads that file, storing the data contained therein (see below).
3. If a PARAMETER\_GROUP\_FILE keyword is present within the WRITE\_PEST\_FILES block, TSPROC reads that file, storing the data contained therein (see below).
4. TSPROC checks that all model entities (ie. time series, s\_tables, v\_tables and e\_tables) cited in the WRITE\_PEST\_FILES block are also cited in the LIST\_OUTPUT block that should immediately precede it in the TSPROC input file.
5. It checks that each observation entity that is matched to a model entity has the same design specifications as its model counterpart.
6. It then generates names for all observations featured in the parameter estimation process (ie. for the individual terms of all time series, and the individual elements of all s\_tables, v\_tables and e\_tables); as is discussed below, these names are based on the names of the respective entities.
7. TSPROC then writes an instruction file by which the "model-generated data" written by the previous LIST\_OUTPUT block can be read by PEST.
8. TSPROC then writes the "control data", "parameter group" and "parameter data" sections of the new PEST control file. Included in this file are all parameters referenced in the template files cited in the WRITE\_PEST\_FILES block. Information contained within the parameter data and parameter group files is included in the pertinent sections of the PEST control file where appropriate. Default values are used for all other PEST variables.
9. The "observation group" and "observation data" sections of the new PEST control file are then written. Observation weights are calculated according to formulae supplied through various WEIGHTS\_EQUATION keywords.
10. The "model command line" and "model input/output" sections of the new PEST control file are then written.

These tasks are now discussed in greater detail.

### Parameter and Parameter Group Data

TSPROC ascertains the names of the parameters that it must include in the PEST control file by reading all template files cited in the WRITE\_PEST\_FILES block. Any number of TEMPLATE\_FILE keywords can be included in a WRITE\_PEST\_FILES block. Optionally, each such keyword can be followed by a MODEL\_INPUT\_FILE keyword. If so, PEST links the cited model input file to the previous template file when writing the "model input/output" section of the PEST control file. If a MODEL\_INPUT\_FILE keyword is not associated with a particular TEMPLATE\_FILE keyword, PEST supplies a default model input filename to correspond to the template file; this filename should be altered to the correct filename in the PEST control file before running PEST.

In writing a PEST control file, TPROC must supply each parameter with an initial value, an upper and lower bound, and all of the other information contained within the "parameter data" section of a PEST control file. It must also assign each parameter to a parameter group. Recall that variables which govern the calculation of derivatives are assigned to parameter groups rather than to individual parameters. For some parameter types, the values assigned to these derivative-calculation variables can be crucial to the success of the parameter estimation process.

If no PARAMETER\_DATA\_FILE keyword is present within a WRITE\_PEST\_FILES block, PEST assigns default values to all parameter variables. It assigns each parameter to a group of its own, and supplies default values to the derivatives-calculation variables pertaining to each such group. The user should carefully inspect all of these variables, altering them as necessary to suite the calibration problem at hand.

If desired, default TSPROC parameter data can be overridden by supplying the values for parameter variables and parameter group variables through a "parameter data file" and a "parameter group file" respectively. The names of these files are supplied following optional keywords of the same name in the WRITE\_PEST\_FILES block.

A parameter data file is illustrated below.

1. Example of a parameter data file.

ro1 fixed factor 0.5 .1 10 ro 1.0 0.0

ro2 log factor 5.0 .1 10 ro 1.0 0.0

ro3 tied\_ro1 factor 0.5 .1 10 ro 1.0 0.0

h1 none factor 2.0 .05 100 h 1.0 0.0

h2 none factor 5.0 .05 100 h 1.0 0.0

For the most part, a parameter data file emulates the "parameter data" section of a PEST control file, containing the same variables in the same order. However, note the following.

1. There is no need to supply a value for the DERCOM variable (the command line number for derivatives calculation - the 10th variable on each line of the "parameter data" section of a PEST control file). TSPROC will always provide a default value of 1 for this variable when it writes a PEST control file.
2. Not all parameters cited in template files need to be cited in a parameter data file. TSPROC will provide default data for parameters that are absent from the latter file.
3. If a parameter is tied to another parameter, the name of the parent parameter must be attached to the "tied" string following an underscore, as illustrated in the above example.
4. If a parameter is assigned to a particular parameter group, and if a parameter group file is not cited in the WRITE\_PEST\_FILES block, or if the name of the group is not included in a cited parameter group file, then TSPROC will supply default values for variables governing derivatives calculation for that group when it writes the PEST control file.

The contents of a parameter group file emulate those of the "parameter groups" section of a PEST control file. An example is provided below.

1. Example of a parameter group file.

ro relative 0.01 0.00 switch 1.5 parabolic

h relative 0.01 1.0e-4 switch 2.0 parabolic

### Time Series Observations

For every time series involved in the parameter estimation process, at least three, and up to four, keywords must be supplied in the WRITE\_PEST\_FILES block. These keywords must be provided in the order presented in the above table.

The time series associated with the OBSERVATION\_SERIES\_NAME keyword should contain measurement data. TSPROC will write the terms of this series to the PEST control file. The goal of the parameter estimation process will be to minimise the discrepancies between these terms and those of a corresponding model-generated time series. The latter will be produced by TSPROC in its role as a model post-processor; as mentioned above, when acting in this latter role CONTEXT settings must be such that a PEST input dataset is NOT generated, and any unnecessary processing of observation data is dispensed with.

The name of the model time series which forms the model-generated counterpart to the observation time series must be supplied with the MODEL\_SERIES\_NAME keyword directly following the OBSERVATION\_SERIES\_NAME keyword. It is important to note that this same series must be featured in the LIST\_OUTPUT block immediately preceding the WRITE\_PEST\_FILES block. This LIST\_OUTPUT block, and all calculations and data importations giving rise to the time series and tables cited in that block, must be retained when TSPROC is run as a model post-processor during the parameter estimation process.

As was mentioned above, a model time series must have identical specifications to an observation time series with which it is paired, both in the number of terms, and the dates/times pertaining to each of its terms. This will ensure that it is valid to compare the two series on a term-by-term basis for the purposes of calibrating a model.

When writing a PEST input file, TSPROC assigns all observations comprised of the terms of an observation time series to a single observation group. This group is given the same name as the model time series to which the observation time series corresponds. Individual observation names are generated by affixing the string "#n..n" to a contraction of the group name, where "n..n" is the term number of the time series. If for some reason this process does not result in unique observation names (which can occur under some circumstances if time series names are too similar), TSPROC will inform you of the problem through an appropriate error message and will then cease execution.

When writing the "observation data" section of a PEST control file, TSPROC must assign a weight to each observation. Observation weights are calculated by TSPROC on the basis of the equation supplied by the user with the WEIGHTS\_EQUATION keyword. The format of the weights equation is the same as that described in the SERIES\_EQUATION block, except for two important differences. These are as follows.

1. If a series name is cited in a weights equation, that series must have the same time-base (same number of terms, and same date/time pertaining to each term) as the observation time series for which weights are being calculated. In implementing the equation for weights calculation, series are matched on a term-by-term basis.
2. An extra TSPROC-specific function is provided for use in a weights equation that is not available for use in a series equation. This is the @\_abs\_val function. This function returns the value of the term of the observation time series for which a weight is currently being calculated.

Some example weights equations follow.

1. Example of valid weights equations.

wt\_series

1.0/sqrt(@\_abs\_val)

4.0

1.0 + 0.5 \* sin((@\_days\_start\_year + 124.5)\*6.284/365.25)

sqrt(@\_days\_"1/1/1989\_00:00:00")

In the first of the above equations, weights are simply equated to the terms of an existing time series (which may have been calculated within TSPROC specifically for this purpose). In the second of the above equations, observation weights are calculated as the inverse of the square root of the absolute value of each observation. In the third example a uniform weight of 4.0 is assigned to all observations comprising the observation time series, while in the fourth example weights show a seasonal dependence, being a function of time of year (note the factor of 2 /365.25 in the argument to the sine function). Recall from the documentation to the GET\_SERIES\_EQUATION block that the argument to the sin, cos and tan functions must be supplied in radians; 2 radians is the same as 360 degrees. In the fifth of the above equations, weights increase as the square root of the number of days that have elapsed since the first moment of 1989.

If any observation weight is calculated as less than zero, TSPROC raises the weight to zero. However the user has the option of supplying upper and lower bounds to the weights him/herself through a SERIES\_WEIGHTS\_MIN\_MAX keyword. (If a user requests a minimum weight of less than 0.0, TSPROC will override this with a minimum weight of zero.)

Note that when generating instructions to read the TSPROC output file whose name is cited in the LIST\_OUTPUT block that immediately precedes the WRITE\_PEST\_FILES block, TSPROC automatically adjusts these instructions according to whether the SERIES\_FORMAT is specified as "long" or "short" in that block. Considerable computation time can be saved if the SERIES\_FORMAT is "short".

### S\_Table Observations

The mechanism by which s\_table observations are included in a calibration dataset is very similar to that by which series observations are included in this dataset. The name of an observation s\_table must be provided through the OBSERVATION\_S\_TABLE keyword. This keyword must be immediately followed by a MODEL\_S\_TABLE keyword through which the name of a corresponding model s\_table is provided. This s\_table must contain the same statistics as those contained within the observation s\_table (statistics for inclusion in an s\_table are requested through the SERIES\_STATISTICS block). This same s\_table must also be featured in the LIST\_OUTPUT block immediately preceding the WRITE\_PEST\_FILES block.

TSPROC assigns all observations pertaining to a particular s\_table to a single observation group whose name is the same as that of the model s\_table. Individual members of the s\_table are provided with observation names by contracting the name of the observation group and appending a shortened form of the name of the statistic which each represents.

Weights for s\_table observations are generated using a weights equation. However unlike the weights equation used in the generation of weights for time series observations, the weights equation used for the generation of s\_table observation weights cannot site a series name. Nor can it use the @\_days\_start\_year or @\_days\_"mm/dd/yyyy\_hh:nn:ss" functions. However it can use the @\_abs\_val function; in this case the value refers to the particular statistical entity contained in the s\_table to which the weight is assigned.

### V\_Table Observations

V\_table observations are included in a calibration dataset in the same way that s\_table observations are included. The only difference is that individual observations are named by affixing a number (rather than a contracted form of the name of a statistical measure) to a contracted form of the observation group name. The latter is named after the model v\_table to which the observation v\_table is matched in the WRITE\_PEST\_FILES block.

### E\_Table Observations

Inclusion of e\_table observations in the calibration process follows the same procedure as that used for inclusion of v\_table observations.

### C\_Table Observations

As presently programmed, data contained within c\_tables cannot be included in the model calibration process. If the name of a c\_table is cited in a WRITE\_PEST\_FILES block, TSPROC will cease execution with an error message.

### The PEST Control File

In the PEST control file written by TSPROC, PEST is asked to run in parameter estimation mode. Default values are provided for all PEST control variables. Fortunately, these are suitable for most occasions; however if a control variable is not suitable for a particular parameter estimation run, it can easily be altered by the user. Similarly, if it is desired that PEST run in another mode, this too can easily be accomplished by direct editing of the PEST control file written by TSPROC. If it is desired that PEST run in regularisation mode, a set of regularisation observations and/or prior information equations must also be added to this file.

If a TEMPLATE\_FILE keyword in a WRITE\_PEST\_FILES block is followed by a MODEL\_INPUT\_FILE keyword, then the model input file is linked to the corresponding template file in the "model input/output" section of the PEST control file. The name of the instruction file recorded in the "model input/output" section of the PEST control file is that which is written by TSPROC, the name of which is associated with the NEW\_INSTRUCTION\_FILE keyword. This is matched to the model output file whose name is provided with the FILE keyword in the LIST\_OUTPUT block immediately preceding the WRITE\_PEST\_FILES block.

If a MODEL\_COMMAND\_LINE keyword is provided in a WRITE\_PEST\_FILES block, the user-supplied command line is transferred to the "model command line" section of the PEST control file written by TSPROC. Otherwise a default command line is used; this will probably need to be altered by the user before running PEST. Note that the model command line will be the name of a batch or script file. Commands cited in this file will include the name of a model executable, as well as the command to run TSPROC. TSPROC’s keyboard responses will need to be written in advance to a small file whose name must be included in the command to run TSPROC following the "<" symbol denoting keyboard re-direction.

The AUTOMATIC\_USER\_INTERVENTION keyword is used to set the DOAUI variable in the "control data" section of the PEST control file written by TSPROC. If this is set to "yes" then DOAUI is set to "aui"; thus PEST will implement automatic user intervention as necessary when implementing the inversion process. If AUTOMATIC\_USER\_INTERVENTION is set to "no", or if it is omitted, then DOAUI is set to "noaui". Note that, regardless of the setting of this variable, TSPROC does not add an "automatic user intervention" section to the PEST control file which it writes. Thus if automatic user intervention is implemented, it is done on the basis of default values for variables which control its implementation. If he/she wishes, the user can easily add this section to the PEST control file him/herself.

An alternative numerical stabilisation device is truncated singular value decomposition (i.e. "truncated SVD"). This is invoked by supplying a TRUNCATED\_SVD keyword, followed by the value of the truncation threshold (PEST variable EIGTHRESH) which is normally between 10-6 and 10-7. Note that TSPROC will object if both a TRUNCATED\_SVD and AUTOMATIC\_USER\_INTERVENTION keyword is supplied, for only one (but not both) of these stabilization devices can be employed at the same time. Note also that if truncated SVD is selected as a numerical stabilization device then the initial lambda (RLAMBDA1 variable) is set to zero and the number of tested lambdas per iteration (NUMLAM variable) is set to 1 in the PEST control file written by TSPROC.

Notwithstanding the fact that it may require some alterations before being used by PEST, a PEST control file written by TSPROC is complete enough to withstand the scrutiny of PESTCHEK. As is described in the PEST manual, PESTCHEK checks both the PEST control file whose name is provided on its command line, as well as all template and instruction files cited within the PEST control file. Because TSPROC uses parameter names found in one or a number of template files in its construction of the PEST control file, and because it generates the instruction file itself for the current parameter estimation process, PESTCHEK should not detect any errors or inconsistencies in the PEST input dataset built by TSPROC (unless these have been introduced through a spurious parameter data file or parameter group file).

### Calibration using "Patterns"

There are some instances of model calibration where the direct matching of raw or processed observation data to corresponding raw or processed model-generated data might not work as well as other strategies for at least some of the data types that may be included in the model calibration process. Certain types of stream quality data fall into this category. For these data types a better calibration strategy may be to attempt to match some relationship between flows and constituent measurements (calculated on the basis of observations on the one hand and model outputs on the other), rather than the individual constituent concentrations themselves. For example the calibration process may attempt to ensure that a regression relationship involving flows, constituent data, and possibly other factors such as time of year, is respected by the model, even if the model is incapable of replicating individual constituent measurements due to the erratic and noisy nature of these measurements.

As an example of the application of this principal, consider that it is "known" that a certain regression relationship exists between flow and constituent concentrations. The coefficients in such a relationship may have been determined through using a model such as the USGS program ESTIMATOR; or they may even have been determined using PEST in conjunction with TSPROC, with the SERIES\_EQUATION block of TSPROC comprising the "model". As part of TSPROC’s model post-processing duties, model-generated flows and constituent concentrations could be time-interpolated to the dates and times at which constituent measurements were made. Using the SERIES\_EQUATION block, the difference between model-calculated concentrations and those "predicted" using the regression equation applied to model-generated flows could be evaluated. The closer that the difference between these two quantities is to zero, the closer does the "constituent pattern" generated by the model match the observed "constituent pattern". (Other factors will come into play here, such as the average and standard deviation of the constituent measurements which, as discussed above, are also easily incorporated into the parameter estimation process.)

In order to incorporate "pattern matching" of this type into the parameter estimation process, a time series expressing the difference between modeled constituent concentrations and those calculated from modeled flows using the "known" regression equation can be supplied as a model time series in the WRITE\_PEST\_FILES block (and the LIST\_OUTPUT block preceding it). For consistency, dates and times for this time series should correspond only to constituent measurement times. The corresponding observation time series would be one with an identical time-base, but with all terms equal to zero. Weights assigned to these "observations" could be uniform; alternatively they could be a function of the actual observed constituent concentrations, calculated using a SERIES\_EQUATION block and supplied through the SERIES\_WEIGHTS\_EQUATION keyword.

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# Appendix 1: Site Sample File

The "site sample file" is fundamental to the operation of many of the Surface Water Utilities; it holds time series data gathered at one or a number of sites. The data stored in this file can be of any type.

A site sample file records data gathered at discrete sample times at a number of specific locations, eg. water level or chemical concentration data gathered through sampling programs. Each line of a site sample file has four (or possibly five) entries, each of which must be separated from its neighbouring entry by one or more white space (including tab) characters. Typically a site sample file will hold data extracted from a database. Part of a site sample file is shown below.

1. Extract from a site sample file.

13500002A 25/09/1991 12:00:00 12.00

13500002A 02/01/1992 12:00:00 11.83

13500002A 24/03/1992 12:00:00 12.81

13500002A 29/06/1992 12:00:00 13.54

13500002A 22/09/1992 12:00:00 13.24

13500002A 17/12/1992 12:00:00 12.84

13500002A 22/03/1993 12:00:00 12.38 x

13500002A 21/06/1993 12:00:00 11.83 x

13500002A 27/09/1993 12:00:00 11.61 x

13500002A 16/12/1993 12:00:00 12.35

13500002A 01/03/1994 12:00:00 11.79

13500002A 22/03/1994 12:00:00 11.89

1351235A 19/02/1959 12:00:00 29.84

1351235A 05/03/1959 12:00:00 30.33

1351235A 20/03/1959 12:00:00 30.76

1351235A 06/04/1959 12:00:00 31.19

1351235A 17/04/1959 12:00:00 31.45

1351235A 01/05/1959 12:00:00 31.65

site\_a 15/05/1959 12:00:00 31.65

site\_a 29/05/1959 12:00:00 31.65

site\_a 12/06/1959 12:00:00 31.65

site\_a 26/06/1959 12:00:00 31.46

site\_a 10/07/1959 12:00:00 31.34

The first item on each line of a site sample file is a site identifier. This identifier must be of 10 characters or less in length. When used with programs of the Surface Water Utilities the site identifier is case-insensitive. The second item is the date; depending on the contents of the settings file settings.fig (see the introduction to this manual), this must be expressed either in the format dd/mm/yyyy or mm/dd/yyyy. Then follow the time (in the format hh:mm:ss) and the measurement pertaining to the cited date and time. An optional fifth item may be present on any line; if present, this item must consist solely of the single character "x" to indicate that the previous data element lacks integrity.

The following rules must be observed when generating a site sample file:

* For any one site dates and times must be listed in increasing order.
* All entries for the same site must be in juxtaposition; in other words, it is not permitted to list some of the entries for a particular site in one part of a site sample file and the remainder of the entries in another part of the same file, with data pertaining to one or more other sites in between.
* A time entry of 24:00:00 is not permitted; this must be represented as 00:00:00 on the following day.

The integrity of a site sample file can be checked using program SMPCHEK documented herein. If any errors are present in a particular file of this type, they will be reported to the screen.

# Appendix 2: Notes for developers

General discussion of object-oriented nature of the current code; example of how to extend in Fortran and in Python.