

**REGIONAL APPLICATION OF THE PITMAN MONTHLY
RAINFALL-RUNOFF MODEL IN SOUTHERN AFRICA
INCORPORATING UNCERTAINTY**

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Dedication

This thesis is dedicated to my parents: my mum, Diana and my late father, Austin.

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ABSTRACT

Climate change and a growing demand for freshwater resources due to population increases and socio-economic changes will make water a limiting factor (in terms of both quantity and quality) in development. The need for reliable quantitative estimates of water availability cannot be over-emphasised. However, there is frequently a paucity of the data required for this quantification as many basins, especially in the developing world, are inadequately equipped with monitoring networks. Existing networks are also shrinking due mainly to shortages in human and financial resources. Over the past few decades mathematical models have been used to bridge the data gap by generating datasets for use in management and policy making. In southern Africa, the Pitman monthly rainfall-runoff model has enjoyed relatively popular use as a water resources estimation tool. However, it is acknowledged that models are abstractions of reality and the data used to drive them is imperfect, making the model outputs uncertain. While there is acknowledgement of the limitations of modelled data in the southern African region among water practitioners, there has been little effort to explicitly quantify and account for this uncertainty in water resources estimation tools and explore how it affects the decision making process.

Uncertainty manifests itself in three major areas of the modelling chain; the input data used to force the model, the parameter estimation process and the model structural errors. A previous study concluded that the parameter estimation process for the Pitman model contributed more to the global uncertainty of the model than other sources. While the literature abounds with uncertainty estimation techniques, many of these are dependent on observations and are therefore unlikely to be easily applicable to the southern African region where there is an acute shortage of such data. This study focuses on two aspects of making hydrologic predictions in ungauged basins. Firstly, the study advocates the development of an *a priori* parameter estimation process for the Pitman model and secondly, uses indices of hydrological functional behaviour to condition and reduce predictive uncertainty in both gauged and ungauged basins. In this approach all the basins are treated as ungauged, while the historical records in the gauged basins are used to develop regional indices of expected hydrological behaviour and assess the applicability of these methods.

Incorporating uncertainty into the hydrologic estimation tools used in southern Africa entails rethinking the way the uncertain results can be used in further analysis and how they will be interpreted by stakeholders. An uncertainty framework is proposed. The framework is made up of a number of components related to the estimation of the prior distribution of the parameters, used to generate output ensembles which are then assessed and constrained using regionalised indices of basin behavioural responses. This is premised on such indices being based on the best available knowledge covering different regions. This framework is flexible enough to be used with any model structure to ensure consistent and comparable results.

While the aim is to eventually apply the uncertainty framework in the southern African region, this study reports on the preliminary work on the development and testing of the framework components based on South African basins. This is necessitated by the variations in the availability and quality of the data across the region. Uncertainty in the parameter estimation process was incorporated by assuming uncertainty in the physical and hydro-meteorological data used to directly quantify the parameter. This uncertainty was represented by the range of variability of these basin characteristics and probability distribution functions were developed to account for this uncertainty and propagate it through the estimation process to generate posterior distributions for the parameters. The results show that the framework has a great deal of potential but can still be improved. In general, the estimated uncertain parameters managed to produce hydrologically realistic model outputs capturing the expected regimes across the different hydro-climatic and geo-physical gradients examined. The regional relationships for the three indices developed and tested in this study were in general agreement with existing knowledge and managed to successfully provide a multi-criteria conditioning of the model output ensembles. The feedback loop included in the framework enabled a systematic re-examination of the estimation procedures for both the parameters and the indices when inconsistencies in the results were identified. This improved results. However, there is need to carefully examine the issues and problems that may arise within other basins outside South Africa and develop guidelines for the use of the framework.

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CHAPTER 1

INTRODUCTION

1.1 Background and Rationale

Effective and sustainable management of water resources demand reliable quantifications of water amount, distribution and quality. With demands on water resources rapidly growing across the globe there is a growing need for accurate monitoring, forecasting and simulation of hydrologic variables especially in the major (often transboundary in nature in southern Africa) river basins, for optimal water resources management and, more urgently, food security. However, the available data are frequently far from being sufficient (both in terms of accuracy and spatial/temporal resolution) for the practical application of the best estimation methods. In many parts of the world, especially in the developing countries, there is a severe lack of historical observations regarding essential water resources variables (WWAP, 2009), rendering many basins effectively ungauged. This usually leads to a considerable gap in the understanding of the components of these vital resources, leading to poor quantification of the resources and impacting decision and/or policy making. In the long run, with the rapid growth of demand for water resources of a reasonable quality, this places a limit on the future human and socio-economic development of the region (Basson et al., 1997). This knowledge gap has been partly bridged by the use of hydrological and water resources models (Oreskes, 2003). These have therefore emerged over the past forty years or so as practical tools to provide the necessary information on water availability and quality, as well as being used to simulate the impacts of present day and future human development. More recently they have also been applied to the problem of predicting the hydrological impacts of land use and climate change and the effects on water resources availability. It is safe to conclude that the science of hydrology over the years has evolved from merely being an observational science to a predictive science (Whitfield et al., 2006).

It is impossible to accurately represent all hydrological processes in a model and the information available to establish a model for any specified basin (i.e. climate and basin physical property data such as topography, soils, vegetation, geology, etc.) is typically less than perfect. This inevitably results in predictions that are imperfect and that could span a range of equally plausible simulations. Uncertainty is an unavoidable element in any hydrologic modelling study (Beven,

2001; Wagener et al., 2004) and the concept of uncertainty is the basic tenet and modelling philosophy advocated by Beven (1993) and is the cornerstone of a ten year initiative by the International Association of Hydrological Sciences (IAHS) on Prediction in Ungauged Basins (PUB, Sivapalan et al., 2003). PUB aims to improve the ability of the hydrological community to predict hydrological behaviour at any given ungauged site. While this is a difficult task which may be difficult to achieve, it is the understanding and treatment of uncertainty in the whole prediction process that may eventually provide insight into the problem of ungauged basins (Meixner et al., 2004). A number of international working groups were established in order to achieve the objectives of PUB and one of these is the Uncertainty Working Group. The Uncertainty Working Group has been tasked with exploring novel ways to explicitly estimate and propagate all possible sources of uncertainty in hydrological modelling and seek a unifying framework for evaluating models under uncertainty (Wagener et al., 2006b).

Notwithstanding the undeniable utility of models in water resources management, it is necessary to explicitly acknowledge the limitations, and often futility, of pursuing optimum solutions based on the use of imprecise representations of reality and forcing data. Model prediction uncertainty has therefore become an integral component of model application. Many questions arise in the use of model outputs in water resources planning and management and one of the most significant is how defects in data and the models affect prediction accuracy and uncertainty. The literature abounds with descriptions and discussions of uncertainty and the three major contributory sources of uncertainty in water resources estimation include the quantity and quality of the input data used to force the model, model structural and parameter estimation errors (Ratto et al., 2007; Walker et al., 2003). One of the ways to address this uncertainty challenge is to improve data collection but this has to be done in relation to current theory, lest resources be expended with little benefit. However, improvements in the theory should also take cognizance of the realities of available and collectable data, otherwise they are unlikely to yield productive results (Sieberstein, 2006).

The use of model-based results in policy and/or decision making makes it imperative to have the 'best' information (in whatever form) to be available for reliable and robust results (Reggiani et al., 2009). If the information available is uncertain and therefore cannot give an accurate and/or optimum basis for decision making, then the level of the uncertainty must be ascertained and acknowledged. This enables a decision maker the latitude to make an informed

choice based on some form of risk analysis. Understanding, quantification and accounting for uncertainties is expected to contribute to improved decision making and thus improved management practices (Ajami et al., 2007). Uncertainty analysis is central to improving the predictive capacity of hydrologic models and uncertainty assessment of model simulations has risen to prominence in the last few years (Refsgaard et al., 2007; Pappenberger and Beven, 2006), while uncertainty reduction is the focus of the PUB (Sivapalan et al., 2003) programme.

One of the critical issues with regards uncertainty in water resources modelling is how to do practical assessments in ungauged basins. In the literature, many reviews and techniques are based on reasonably gauged basins and little is said about the ungauged basins. It is important to realize and accept that historical observations are only available for a limited number of basins and the majority of the basins globally are ungauged. This means that there is an urgent need to develop techniques for accounting for uncertainty in such situations. This is not an easy undertaking as there are no data to guide predictions, making it effectively impossible to accurately quantify the confidence in whatever methods may be developed. A number of approaches to modelling based on uncertainty have been proposed and used in PUB with the aim of making predictions in ungauged basins. The basics have been to try to account for the various sources of uncertainty and include the generation of all acceptable possible model outcomes covering the expected range of uncertainty as well as regionalization (Nathan and McMahon, 1990) methods. The latter are difficult approaches to use in a region like southern Africa where the data available are usually insufficient for the establishment of local models (i.e. calibration process) which is the first step in developing regional relationships. However, the transition from the identification of local models at gauged basins to the establishment of relationships for regional models suitable for ungauged sites has some significant shortcomings related to the uncertainties associated with the local models and how these are affected by data errors and their own parameter uncertainties (Wagener et al., 2004; Wagener and Wheater, 2006). It should be noted that the streamflow data available in many regions are the residual flows after poorly- or un-quantified upstream human developments, which means they would rarely represent natural hydrology conditions. Even the regional calibration approach by Fernandez et al., (2000), which simultaneously optimizes both the model parameter calibration and the regional relationships, is unlikely to be effective in such situations.

Alternatives have been based on the generation of an ensemble of predictions for ungauged basins (e.g. Wagener and Wheater, 2006, McIntyre et al., 2005 and Yadav et al., 2007), or the use of *a priori* parameter estimation techniques (e.g. Koren et al., 2004; Kapangaziwiri, 2008). The latter approach avoids reliance on historical data for calibration of the model. This study explores the combined use of two approaches used in PUB for the generation of ensemble predictions for the ungauged basins of southern Africa. *A priori* parameter estimates are generated based on available basin physical property data. Conceptual relationships between the model parameters and basin physical and/or hydro-climatic data are developed based on general physical hydrology principles (Kapangaziwiri, 2008). To be able to generate output ensembles, prior probability distributions are developed for the parameters which account for the uncertainty expected in their determination. The uncertainty distributions are developed through the incorporation of the variability in the basin physical data (Chapter 4). Simple sampling from the feasible parameter space results in sets of parameters that are used to generate multiple outputs. What is therefore required is to determine the limits of acceptability for the outputs in order to reject the unacceptable models. One way of doing this is to explore the use of characteristics of catchment hydrological behaviour to assess and condition the model simulations. The question that needs to be answered is 'are there data available to develop such behavioural indices (or footprints)?'. These indices could possibly be determined from relationships with physical basin attributes (predictors). A simple example of a catchment hydrological response index is the runoff coefficient which would require such data as mean runoff and mean precipitation. In order to include all the possible values of the index, there is need to incorporate the uncertainties related to its estimation and the task is to explore how this could be achieved and determine the limits of acceptable uncertainty.

In a region such as southern Africa, there has been a long history in the use of models for regional and national water resources assessments and the solution of practical problems and one of the tools extensively used is the Pitman (Pitman, 1973; Hughes et al., 2006), conceptual, semi-distributed monthly rainfall-runoff model. In South Africa, the model is applied at the so-called quaternary sub-basin (or catchment) scale (from 10's to over 10 000 km² of area). Application of the model in ungauged basins has been based on regionalized parameter sets. While these sets have worked well in some basins, there are basins in which they have produced less than satisfactory results. It is well accepted that there are uncertainties related to both the parameterisation of the model and

regionalization process. However, regional water resources assessments have continued to be used in water resources planning and management without any explicit incorporation of uncertainty, regardless of the results being based on regional extrapolations from very limited observed data. South Africa has had water resources assessment studies since the 1970s, with the most familiar being the water resources assessment project of the early 1990s (WR90, Midgley et al., 1994) and the more recent WR2005 (Bailey, 2009). There are many instances where updated simulations have been used for specific basins and the results are often very different to the WR90 or WR2005 data. While such a situation points to potential problems in the regional application of the model and represents a clear example of the existence of uncertainty, the uncertainty is never quantified. Earlier recognition of the uncertainty problem in water resources assessment can be found in Ashton et al. (1999) and Anderson (2002). These articles allude to the uncertainty inherent in assessment tools used in South Africa and the potential impacts of this on model outputs. Experience of water resources estimation in the country (and within the region) also suggests that there is some skepticism about modelling outputs and an acknowledgement of uncertainty within the hydrological community. Currently, new results (e.g. WR2005) are simply used as the 'best available' data (unquestioned conventional wisdom!). There is therefore no framework to either quantify uncertainty or use it in the various decision making processes. There are likely to be other situations around the world where similar problems exist. It has been argued elsewhere in this thesis that quantification of uncertainty should lead to increased information for the decision maker, and more reliable outputs. It is also prudent to note that unless uncertainty is properly incorporated and quantified, it will be difficult to properly understand the reliability of model results and model-based decisions.

The science of the natural environment is an uncertain science. Practitioners cannot make predictions for practical problems without significant uncertainty in representing the processes involved. In catchment management, this inherent uncertainty is exacerbated by the additional complexities of future climate change. The complexity and uncertainty inherent in water resources estimation tools ought be considered and managed in an appropriate manner for increased confidence in model-based decisions. Beven (1989) has pointed to the limitations of the current generation of rainfall-runoff models and argued that the possible way forward must be based on a realistic assessment of predictive uncertainty. To adequately address uncertainty in hydrologic modelling, there are three distinct

yet related aspects to be considered: understanding, quantification, and reduction of uncertainty (Vrugt et al., 2005). While many uncertainty analysis tools exist internationally, it is also prudent to accept that the majority cannot be laterally transferred into the region without substantial modification. It is therefore imperative to develop 'local' methods suitable for the data conditions (quality and accuracy) and assessment tools obtaining in the region. Public discourse and policy decisions within the region are shaped by model results without consideration of the uncertainties inherent in these results since stakeholders usually contend that total accuracy is not a pre-requisite for decision making. However, quality and utility of model-based decisions are enhanced by incorporation of uncertainty. A consideration of uncertainty and its proper communication to both decision makers and stakeholders should improve those model-based decisions. This study therefore investigates the incorporation of parameter estimation uncertainty, one of the important sources of uncertainty in the generation of stream-flows using the Pitman model. It also hoped that the protocols for uncertainty incorporation developed in this study will be flexible enough for use with different model structures and, therefore, provide a consistent framework for model application and/or analysis in the region. The procedures developed in this study should contain a common platform for model application and produce consistent outputs. This study therefore attempts to contribute to the discourse on bridging this information gap and improving water resources assessments and decision making in the region.

1.2 Research questions of the study

This study is guided by, and seeks to provide answers to, the following two sets of questions:

- How can models provide useful information that can be successfully used for decision making in southern Africa given the data scarcity situation?

This is the primary question that seeks to address model prediction uncertainty quantification in the face of inadequate data which is a typical problem in many basins in the region. The aim is to incorporate this into the decision making process. Notwithstanding data shortages, water-related developments still have to take place for social and economic development. The risks associated with this approach are unknown but there are real chances of sub-optimal use of resources

based on conservatism in planning. This is one example of decision making using imperfect information. It is therefore imperative that the information content of model results be improved and one way of achieving this is by incorporating the uncertainty into the modelling process. Such an approach would reveal the limitations of scientific understanding and the data used to guide the modelling process and inform the extent of confidence that can be expressed in the outputs.

The secondary question, which is a corollary of the first, is:

- What is the best approach for regionalizing water resources assessments in ungauged basins in southern Africa that will help to achieve a harmonized and consistent water resources management framework?

This secondary question recognizes that the assessment of water resources in southern Africa has been based on many tools, most imported from outside the region. The results of these studies have at times been difficult to collate especially given the diversity of tools that have been used. From the Flow Regimes from International Experimental Network Data (FRIEND, Hughes, 1997) project it is clear that, while it is acknowledged that such studies existed, access to the results was often difficult. This study therefore chooses to use the Pitman (Pitman, 1973; Hughes et al., 2006) model which has been used extensively throughout the region since its large scale introductory application outside South Africa. Since then the Pitman model has enjoyed relative success in simulating the vast ranges of physical conditions obtaining in the region.

The subsidiary questions that will support this secondary question, and related specifically to the Pitman model, are:

- Can model parameters be defined in a physical manner that is consistent with physical hydrology principles? If so, what relationships exist between the parameters and the physical basin characteristics?
- What appropriate sources of data can be used to aid the parameter estimation procedures?
- What are the major sources of uncertainty in the parameter estimation process and what is the result of local model parameter estimation uncertainty on the regionalization result?
- How is local parameter uncertainty propagated into predictions in ungauged basins and what is the result? What ranges of physical basin property details give acceptable ranges of hydrological output?

- How can the results be used to develop guidelines for the application of the model?

1.3 Aims and Objectives of the study

The intended ultimate goal of a study of this nature is to contribute to the development of an uncertainty framework for the application of the Pitman rainfall-runoff model that includes *a priori* parameter estimation and that can be applied in any basin, gauged or ungauged, in southern Africa. This study will produce a revised and improved parameter estimation protocol that directly incorporates uncertainty for use in southern African basins under different climate, topography, geology, soils, vegetation, data availability and data quality conditions. The key is to develop parameters that produce levels of model output uncertainty that can be useful in decision making. Thus, based on the questions outlined in section 1.2 and the overall aim stated herein, the specific objectives of the study are:

- To develop and test parameter estimation procedures for the parameters of the Pitman model.*** This study is a component of the author's ongoing research and part of the work on parameter estimation procedures for some of the parameters of the Pitman model was tackled as part of a Master of Science (MSc) project (reported in Kapangaziwiri, 2008). The previously developed procedures parameters were for the soil moisture accounting (ST), runoff (FT, POW), recharge (GW, GPOW) and infiltration (ZMIN, ZMAX) components and were successfully tested in many basins in southern Africa. The results showed that the conceptual framework and the estimation principles used for the development of the parameter estimation procedures were robust and hydrologically sound. The simulations were successful in all basins tested in South Africa, Botswana, Mozambique, Zambia and Zimbabwe. Based on these encouraging results, a decision was taken to extend the same estimation principles to the remainder of the calibration parameters of the model.
- To identify appropriate sources of physical property basin data available in the region that can be used for parameter estimation.*** There are various sources of data that can potentially be used in a study of this nature. However, the aim of the study is to identify information sources that are readily available in many parts of the region without the need to invest heavily on resources to acquire new data. Such information

pertaining to, *inter alia*, geology, relief, slopes, soils, evaporation and rainfall estimates are generally available in the region and can be used as a basis for development of the methods. It is recognized that the same types of information will not be available consistently across the region and that the level of detail and quality of the available data will vary. Differences in detail and quality are therefore expected to contribute to the uncertainties in the data used in the parameter estimation process, which leads to the next specific objective.

- iii. ***To develop procedures to include uncertainty into the parameter estimation process.*** These procedures are expected to take cognizance of the fact that the estimation equations are not perfect and neither are the input physical property data. The *a priori* estimation methods pursued in this study are expected to be affected by the quality and detail of the basin physical data that are available. Identification of the various potential sources of error is important in determining the level of reliability in the parameters and the resultant model simulations, and the design of possible intervention measures such as improved data collection methods.
- iv. ***To assess the uncertainty in the parameter estimation process by comparing model outputs with alternative measures of catchment behaviour response.*** It is expected that some measure of catchment functional (or response) behaviour will be developed to condition model outputs in the absence of observed flows. The rationale is that if the approach is to work for ungauged basins there has to be a control for assessing model performance, a function which is performed by observed flows in the case of gauged basins. Without such a model conditioning criterion, it would be difficult to accept and/or reject any model outputs in an ungauged basin and the approach would inevitably fail.
- v. ***To carry out a comprehensive assessment of the uncertain parameter estimation process using sensitivity analysis and to identify where improvements are required in the estimation process.*** The sensitivity analysis is essential to test some of the underlying assumptions of, and the process representations in, the parameter estimation processes. The sensitivity analysis is expected to be simple and used to identify the parameter variations across different conditions (e.g. climate zones) for feedback to the estimation process.
- vi. ***To make recommendations about the use of the proposed uncertainty framework for the Pitman model and where further work has the potential to improve the approach.*** The idea is to

assess how the Pitman model can be used in the proposed uncertainty framework. It is expected that some components of the framework may need improving or that the Pitman model may not work well in some areas. These will need to be highlighted wherever possible so that necessary future efforts can target these for improvement.

1.4 The study area

The ultimate intention of the study is to cover the southern African region. Part of the motivation is that the sub-region needs to adequately ascertain its water resources availability, and with increasing demand on water resources expected in the future such a study is imperative for planning, management and development purposes. With the exception of South Africa, the current information on water resources availability in the region is at best piece-meal, and covers only a relatively small gauged part, with very little being known about the resource in the ungauged basins. Where such information is available, experience has shown that this has been derived from a multiplicity of methods which makes common understanding and interpretation of results very difficult. Also the region hosts a number of trans-boundary river basins which demand commonality in resource assessment techniques/criteria and negotiated decision making. A common understanding is therefore a prerequisite to a region-wide water resources assessment exercise to achieve the objective of the Regional Water Sector Programme of SADC for “equitable and sustainable access to water resources - improvement in regional integration and economic benefits for present and future generations of southern Africa” (<http://www.sadcwater.com/index.php>). The reliability of the model predictions also needs to be improved so as to curtail liabilities due to conservative over- or under-designing. Water resources decisions in the region are frequently based on model outputs whose uncertainty has never been quantified nor analysed. Given the large disparities in data availability and quality across the sub-region, the development of the uncertainty framework reported in this study will initially be based on datasets from South Africa with the intention of extending the work to other parts of the sub-region later.

Brief description of the southern African region

The climate of the southern African region is very diverse with arid conditions experienced along the western ring (in Botswana and Namibia), and more humid temperate sub-tropical conditions in the south-western and north-eastern parts of

South Africa, northern and western Mozambique, eastern and central Zimbabwe, north-western Zambia, Northern and Central Democratic Republic of Congo (DRC) and central Malawi. The mean annual precipitation (MAP) and the mean annual evapotranspiration (MAE) indicate the diversity of climate (Figure 1.1). Figure 1.1 shows that the spatial distribution of precipitation is not even, with a steep gradient from north to south and from east to west, with South Africa, Botswana, Namibia and Zimbabwe receiving an annual total of less than 800 mm.

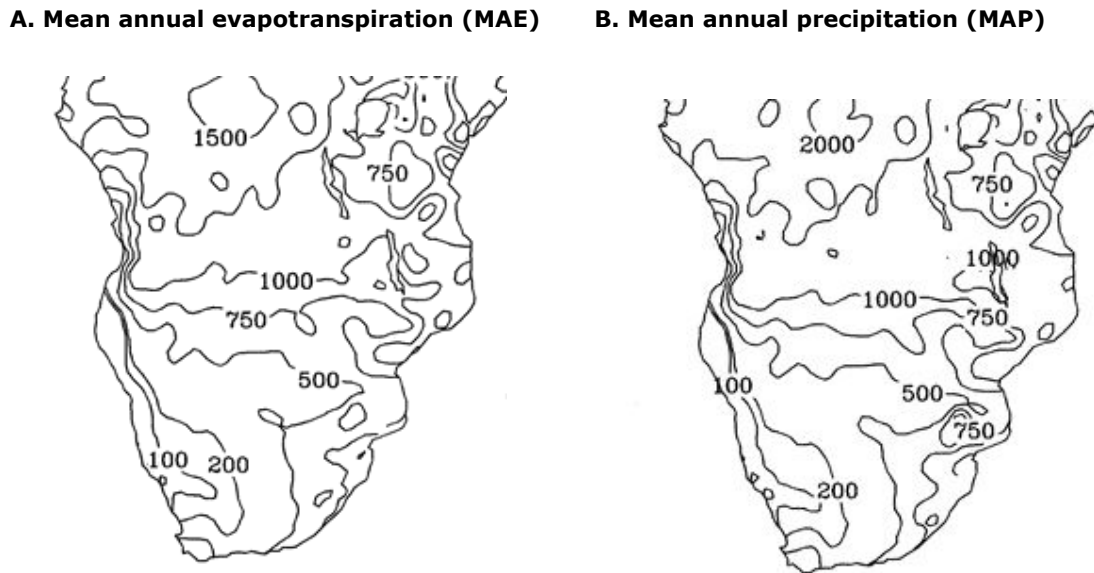


Figure 1.1 The distribution of mean annual evapotranspiration (MAE) and mean annual precipitation (MAP) over southern Africa. The MAP is based average data for the period between 1950 and 1989, (Nicholson et al., 1997).

The runoff coefficient for the region is generally quite low, except for the central parts of the Congo River basin in the DRC. Southern Africa's hydrological regime is characterized by high variability and low runoff coefficients with less than 15% conversion of mean annual precipitation (MAP) to mean annual runoff (MAR) known to be present across large parts of the region (Walmsley, 1991). The relief of southern Africa is equally varied from relatively flat, near sea level areas (in the coastal areas of Mozambique, Namibia, Angola, Tanzania and Mozambique) through undulating topography (in Zimbabwe, Botswana and Central DRC) to steep topography basins in the mountain areas of the region.

Geologically, most of the region is underlain by an assortment of Precambrian formations which are quite deeply weathered, or substantially fractured, rocks of volcanic and metamorphic origin and also large portions of sedimentary rock formations. For instance, from the 1:1 000 000 geological map of Zimbabwe (Rhodesia Geological Survey, 1971) most of Zimbabwe is covered by massive granites of the gneissic form, while most of the Kafue River system flows on granitic forms of one description or other (Burke et al., 1994). The other major forms of geology in the region are the Karoo and Transvaal groups of sedimentary formations consisting of inter-bedded sandstone, shale and mudstone. For example, the coastal low lying parts of Mozambique (Direccao Nacional de Geologia, 1983), Western Angola and Eastern Botswana are lowland sedimentary basins, as are the North-Eastern and Western portions of South Africa which are derivatives of the Karoo system. At the other end of the spectrum are portions of the region that are underlain by one type or another of the metamorphic rock forms, e.g. the ultra-metamorphic rocks in North-Eastern South Africa (where the Sabie river flows, Department of Mines, 1970) and the mafic or acid meta-volcanics or meta-sediments of the central, northern and eastern parts of Zimbabwe (Rhodesia Geological Survey, 1971).

The Food and Agricultural Organisation (FAO, 2003) soil maps show that gypsisols and ferralsols quite dominate the substantial part of the region (Figure 1.2). The former cover portions of South Africa, Namibia, Botswana and Angola, while the latter cover substantial portions of Zambia, Malawi and the DRC. Gypsisols are soils with an accumulation of secondary gypsum and ferralsols are deep, strongly weathered soils with chemically poor, but physically stable subsoil (FAO, 2003). The other soil types in the region are lixisols covering a large part of Zimbabwe and Mozambique, durisols (Western South Africa and eastern DRC) and planosols, covering some eastern parts of South Africa, and some gleysols in the western parts of Zambia and northern DRC. Lixisols are described as soils with subsurface accumulation of low activity clays and high base saturation, while durisols are silica rich soils. Planosols are soils with bleached, temporarily water-saturated topsoil on slowly permeable subsoil and gleysoils are saturated at the surface (FAO, 2003).

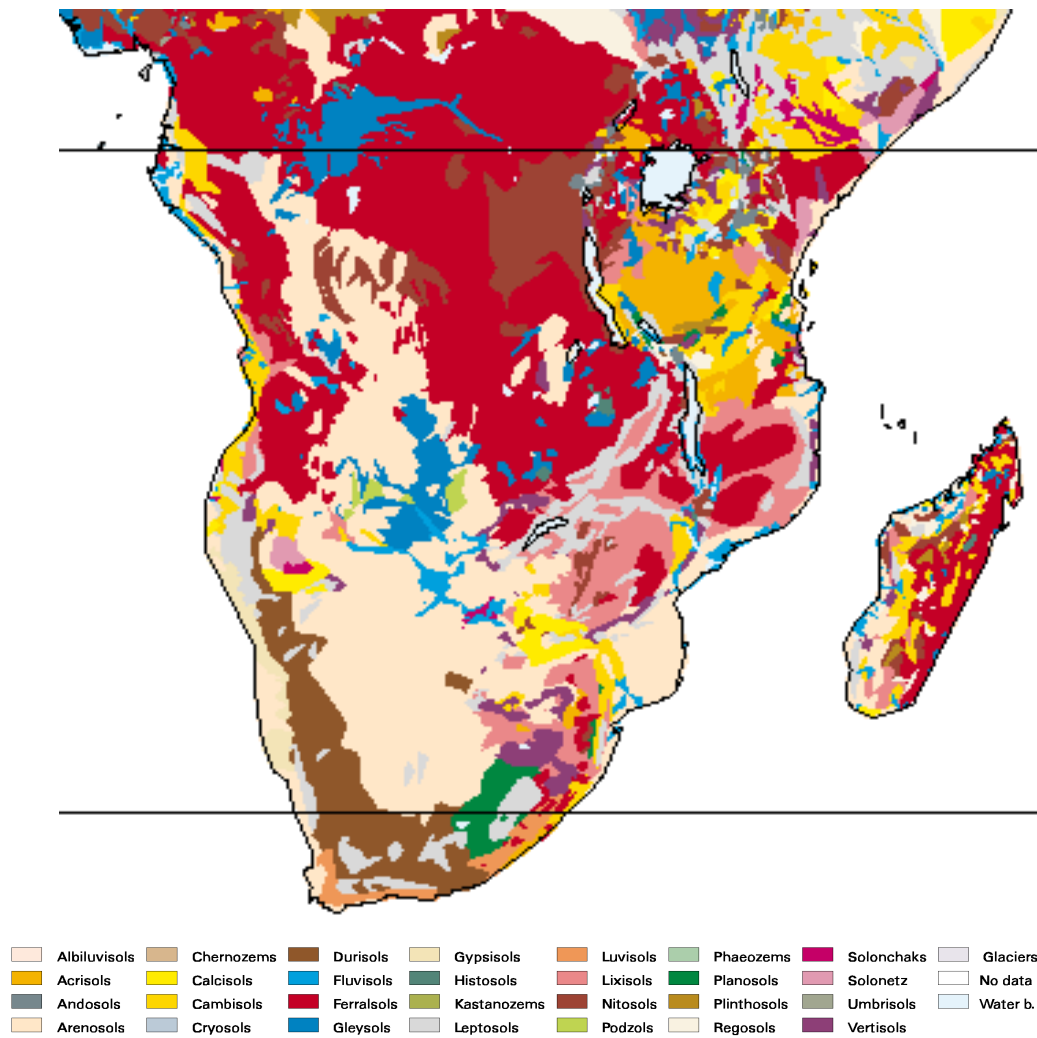


Figure 1.2 The distribution of soils distribution in southern Africa (FAO, 2003)

1.5 Structure of the thesis

Beyond this introductory chapter, the theoretical background on the uncertainty related to hydrological predictions in ungauged basins is covered in **Chapter 2**. **Chapter 3** introduces a framework of incorporating uncertainty that is proposed for southern African basins. The development of the parameter estimation procedures and the incorporation of uncertainty into these procedures are fully described in **Chapter 4**. **Chapter 5** discusses the development of the indices of hydrological behaviour that are used to condition model simulations in an

uncertainty framework. A number of tools, either new or modifications of existing ones were developed to support the framework and are described in **Chapter 6**. **Chapter 7** is a presentation and discussion of the results of the study based on selected South African sub-basins. The overall conclusions and recommendations are summarized in **Chapter 8**.

CHAPTER 2

HYDROLOGICAL PREDICTION UNCERTAINTY IN UNGAUGED BASINS

2.1 Introduction

Rainfall runoff modelling has grown in leaps and bounds since the late 1960s and early 1970s. These periods experienced a growth in model building buoyed by the advent of computers. Consequently, our ability to numerically model natural systems has progressed enormously over the past few decades (Oreskes, 2003). Allied continuous developments in computational power have resulted in the capability to consider and model more detailed and fine resolution processes (Silberstein, 2006). However, it is necessary to take stock of the development of the science of hydrology and hydrological modelling and evaluate the progress (or lack thereof) that has been attained to the present day. This is necessary for two reasons. Firstly, the issue of ungauged basins has brought to the fore the importance of data. For purposes of economic and social development, it has become increasingly significant to forecast water quantity and quality at all scales from the local (point) to the regional (meso and macro) scale including areas where data are not available. This has made regionalization one of the major issues in hydrology. The other reason is more concerned with the development of hydrology as a science and the improvement of our understanding of natural phenomena. The philosophical basis of the modelling approach is the desire to describe the processes in as physically-realistic a manner as possible, given the availability of data (Oreskes and Belitz, 2001; Dornes et al., 2008) and, thus, discover general laws and principles that govern these phenomena. Models are therefore complex assemblages of multiple hypotheses of environmental processes whose utility needs to be established against available data (in Gupta et al., 2008). Methods to evaluate and test these models must be diagnostic in nature (i.e. must provide insight into the degree of realism achieved by the representation and direction as to possible improvements necessary for the model, Gupta et al., 2008) if any hydrological learning is to take place. In many cases such an approach would favour the construction of more parsimonious models, with fewer components and number of parameters. This is, however, at variance with some practical applications that demand detailed process representations capable of responding to environmental setups that are not only complex but do not lend themselves easily to lumping. Whatever the

representation taken for environmental processes, the preservation of physical hydrology principles in hydrological modelling cannot be over-emphasized (Kapangaziwiri, 2008). After forty years of model development, it is clear that within the hydrology community, in spite of all the complex models available, there are still significant gaps in the knowledge of the rainfall-runoff transfer processes (Wagener et al., 2004). This is mainly because of constraints of knowledge and computing capabilities, limited measurement techniques, scale at which measurements are taken (which is different from the scale at which they are required for application) and observational limitations of some processes (Beven, 2002; 2006). This has resulted in most models, notwithstanding the degree of sophistication, being essentially black box in nature with a higher degree of conceptualization than physical basis (Oreskes, 2003; Montanari, 2004). In many cases the same inputs do not result in the same outputs for different models, which compromises their global applicability. On the other extreme, very different values for the same property are necessary for different models even in the same locality. This kind of attribute makes modelling a precarious tool especially in the hands of inexperienced users. It is also a fact that model performances in ungauged basins have been less than satisfactory or reliable. Nash and Sutcliffe (1970) once remarked that "few hydrologists would confidently compute the discharge hydrograph from rainfall data and the physical description of the catchment" and that "this is a practical problem" (pp. 282) that hydrologists face in the field. These sentiments still carry some weight to this day.

While the foregoing assessments about modelling are quite negative and pessimistic, they are a necessary reality check on, and one view of, the science of hydrological modelling over these past few decades. A more optimistic view is to accept the consoling realisation that contemporary hydrologists are better placed with regards hydrological modelling (development and application) than the pioneers (Oreskes, 2003). This has made it possible to make more satisfactory predictions and reliable forecasts. In addition, the science that is coming out of the prediction in ungauged basin (PUB, Sivapalan et al., 2003) initiative is giving tremendous hope to the hydrology community with respect to making predictions in poorly gauged basins. There is a concerted effort to develop new approaches that enable the construction of hydrological models that can be used for making predictions in both gauged and ungauged basins. The basis is that if a model is able to reflect the essence of hydrologic catchment functioning (for the full range of possible states), then it is possible to extrapolate with a higher degree of

confidence beyond the observed conditions and produce reliable predictions (Sivapalan, 2005). Admittedly, a lot of work needs to be done but the current crop of literature points to better methods being developed (for example Beven and Binley, 1992) to achieve reliability for practical and decision making purposes. However, the major problem affecting prediction in ungauged basins is that contemporary approaches are dependent to a great extent on regionalization, which is severely handicapped by several limitations (Yadav et al., 2007). Chief among these is the dependence of regionalization on calibration in a number of gauged basins in order to establish relationships between calibrated parameters and basin attributes. In a region like southern Africa, there are inadequate data for such calibration. This highlights the importance of observations and lends credibility to the argument that decision making in, and management of, water resources does not depend on complexity of models (or the improvement of current models) without improvements in data collection because it is difficult to manage what has not been measured (Silberstein, 2006). This makes regionalization unlikely to work and demands that, while plans to boost measurement networks to (at least) the primary network levels, scientists develop methods that provide a way around dependence on calibration. It would be desirable if such methods would make use of incomplete (lots of missing data) and short observed historical records (both of which are not useable for normal calibration) that may be available in the region.

One of the problems that has not received a lot of attention when considering modelling is the experience of the model developer and, especially, the user. In general it is true that for any relevant and sensible decision making, the use of models must be complemented by sound scientific judgement based on field experience and/or observations. It is thus imperative that a model user has sufficient background in hydrology (and perhaps modelling?). This is necessary to ensure that the user is cognizant of the limitations of the model they are using and also the hydrologic complexities of the field conditions in the basin under study (Anderson, 1983). Anderson (1983) contends that institutionalized 'black-boxing' of models without this education to gain the necessary experience could be hazardous. This quotation from Anderson aptly summarises the importance of a sound grounding in hydrology; "Applying a model is an exercise in thinking about the way a system works. Automating a modelling exercise to the extent that the model can be used by someone lacking the necessary background in hydrology destroys the essence of modelling. It is the thought process needed when applying a model that should lead to a decision, not necessarily and

certainly not exclusively the answers generated by the model itself". The model, regardless of sophistication, remains a tool that can be manipulated to aid decision making. Also, successful model development depends on a clear understanding of the hydrologic conditions of the field area, lack of which often leads to models that are based on inappropriate assumptions of what actually occurs in the real world (Watson and Burnett, 1995). This is one of the major sources of uncertainty which, fortunately, can be addressed quite easily. However this is a problem in Southern Africa where resources (both human and financial) are in short supply (Hughes, 2004b).

In the endeavor to make precise predictions of river flow in any ungauged basin (and a huge amount of basins the world over are virtually ungauged), there is muted consensus in the hydrology community that such a feat may never be accomplished (Meixner et al., 2004). However, what has emerged as a significant constituent to the understanding of the problem of making predictions in ungauged basins is how uncertainty ought to be treated (Chapter 3). A better understanding of uncertainty is likely to result in better interpretations of the resulting model predictions, regardless of the data situation of the basin. Thus, it has become a focus of hydrological modelling to investigate the possible sources of uncertainty, quantify this uncertainty and assess its impact in hydrologic predictions. The philosophy being employed here is that hydrological flux predictions are impacted to varying degrees by uncertainties and an understanding, and more importantly, a reduction of this uncertainty should lead to better, consistent and more reliable predictions.

2.2 Uncertainty

2.2.1 Introduction

The science of hydrological modelling is a discipline in which considerable uncertainty is inherent. Over the past two decades, in response to the increasing need to make predictions in ungauged basins, it has become unavoidable to consider uncertainty in hydrological research. Beven (1989; 2002) discusses the shortcomings of the current rainfall-runoff models and argues that, to take the science forward, hydrological modelling has to be based on a realistic assessment of predictive uncertainty. According to Chow (1979), uncertainty can be defined as the occurrence of events that are beyond man's control. Uncertainty is a

measure of the 'goodness' of a result. Without such a measure, it is impossible to judge the fitness of the value as a basis for making decisions relating to scientific excellence (Refsgaard et al., 2007; Montanari and Brath, 2004; Montanari, 2007). It is caused by a number of fairly typical factors which are discussed in Section 2.2.2. Uncertainty can be classified into stochastic or epistemic uncertainty (Walker et al., 2003). The former refers to the uncertainty related to the natural variability or randomness inherent in all environmental systems. Natural phenomena are influenced by random variability which is usually reflected in historical observations. This variability is irreducible irrespective of advances in measurement technologies. In water resources projects it is a common practice by engineers to adopt design floods whose return periods are greater than the design lives of the project in an attempt to accommodate this type of uncertainty. On the other hand epistemic uncertainty is related to the quantity and quality of the knowledge (both data and processes or systems) available. These quantities can be improved by more research and advances in measurement techniques to acquire more and better (e.g. higher resolution) data. Thus, epistemic uncertainty can be reduced. One of the issues related to this class of uncertainty is that even where perfect processes and system knowledge exist, other factors may come be important especially in modelling, e.g. it may not be possible to parameterize the model to sufficiently account for all the possible system conditions irrespective of the 'perfect' model. However, there are processes that hydrologist know very little about and may never be able to know (Beven, 2006). This makes epistemic uncertainty an integral part of environmental modelling.

In the discussion of uncertainty it is prudent to distinguish between uncertainty and variability, as these two are not synonymous. Variability is an inherent property of the constituent physical system and model components and it cannot be reduced by collecting more data. This can only be quantified by statistical analyses of data collected from the system. On the other hand, uncertainty is usually a limitation imposed by a lack of knowledge. Some uncertainties in variables or systems can be reduced (but rarely eliminated), either by improving the methods of measurement and analysis or by improving the formulation of a model. There are many reasons why modelling uncertainty has dominated attention in the hydrology community such as:

- ❖ The paucity of data due to financial and time constraints
- ❖ Heterogeneity of the earth surface leading to variations of some components or processes through many magnitudes over relatively short distances.

- ❖ The failure to achieve unique optimum model simulations through calibration with many different parameter combinations and conceptual models successfully reproducing observed response. This is the problem known as equifinality (Beven, 2001).
- ❖ The disparity in the scales (both temporal and spatial) of model operation and process observation unavoidably leads to averaging and therefore loss of physical integrity of models.

Uncertainty is important in modelling as it can be linked to such concepts as reliability, safety, risk-based design, etc. One needs to appreciate that uncertainty *per se* is not something negative but it turns into something negative when scientists and/or water practitioners fail to estimate or take it into account (Kinzelbach et al., 2003). This emphasises the utility of uncertainty assessments in decision making by water resources practitioners.

2.2.2 Sources of uncertainty

There are many different stages in the model-based water resources assessment process at which uncertainty manifest. From Melching (1995), Walker et al. (2003), Brugnach et al., (2008) and Gupta et al. (2005), the potential sources of hydrological modelling uncertainty can be summarised as the following:

Input uncertainty (quantity and quality): The data used to force the model (e.g. rainfall and evaporation) and for calibration (e.g. river flow) are almost always imperfect due to measurement errors. These imperfections pervade the model application and parameterization process. Input uncertainty is not only a result of spatial heterogeneity (Brugnach et al., 2008). Errors in empirical observations (both random and systematic errors) usually lead to significant differences that may exist between the real value of a quantity and the one eventually used in the model. For reasonably reliable model results, the reference time series of river flows should span the whole spectrum of possible hydro-climatic conditions (i.e. wet and dry, high and low flow periods, etc). Without such coverage (associated with shorter time periods) it would be impossible to account for all the possible model responses and therefore get appropriate parameter values. However, while the issue of data length necessary for parameter identification is important (Gorgens, 1983), the requisite length is inevitably a product of data quality, complexity of the model and climate variability (Yapo et al., 1996). Besides the adequacy of the modelling data, the quality of these data is also important. Data

that have a lot of missing values, whatever their length, are not suitable for use in modelling (Mazvimavi, 2003) and will increase uncertainty in the parameter estimation process. The impact of missing data depends on the loss of information on the time series data. There is also an impact of the temporal resolution of the model on its parameterization which suffers would suffer if there is significant loss of information due to missing values. Notwithstanding advances in data collection platforms and model construction due to better process understanding and improved computing power, input uncertainty is expected to continue to be significant in hydrological modelling due to the high spatial and temporal variability of precipitation which are not easy to adequately incorporate (Kavetski et al., 2006).

Context and framing: The context of any modelling exercise is determined at the initial stages of any project, even before a structure is chosen. This identifies the problem to be solved. There is therefore potential uncertainty associated with the subjectivity incorporated in defining the modelling activity. This is influenced by the experiences, interest and values of the modeller. In many cases, there is also the influence of ambiguous and conflicting knowledge, where information could be understood with different meanings or may explain contradictory facts. Often a lack of consensus in theory may result in uncertainty related to the context and framing of models (Brugnach et al., 2008).

Model structure uncertainty: this relates to the uncertainty associated with the model form and is caused by incomplete understanding and simplified descriptions of modelled processes as compared to reality. Models, by their nature, are simplifications of the complex reality and there are bound to be gaps and compromises in knowledge and the representation of process (Beven, 2001) and their parameters are, in most cases therefore, just effective averages over a large area which is an integral of several processes and their variability (Bergstrom, 1991). Even assuming a perfect observed response at the sub-basin outlet, it would still mean that the model structure would produce uncertain parameters. This is due to the complexity and variability of environmental systems. The resultant unpredictability makes model applications sensitive to boundary and initial conditions. There is an element of subjectivity in the development of a model structure. Ignorance (inadequate, imperfect information) is another influence on model structure. Beven (2002; 2006) contends that there are aspects of environmental systems (for example subsurface flow movements) that hydrologists are not confident about. Process representation of these aspects

in models is bound to be less than perfect, requiring calibration to match to observations. In reality it is also possible to get different parameter values (by calibration) for the same physical property from different model structures in the same basin. This underlies the significance of model structure (and underlying principles, modelling philosophy and assumptions) in conditioning the parameterization of a model. This is irrespective of the complexity of the model and claims of models being guided by physical principles. In this study a single structure is used since it was not part of the project objectives to assess uncertainty due to the model structure. The model structure uncertainty will therefore be assumed to be systematic. However, it is acknowledged that this will not always be case, especially where response characteristics change through time, or between catchments when comparing uncertainties between different catchments.

Model technical uncertainty: Operationalising the conceptual model (Beven, 2001) requires the development of necessary mathematical equations which will be transferred into a computer code. This uncertainty therefore refers to the uncertainty arising from development of a relevant computer code to implement the model. Uncertainty could therefore be a result of inevitable numerical approximations, resolution in space and time and bugs in the software.

Parameter uncertainty: This relates to the inability of the model structure to locate a unique optimum (or 'best') parameter set given the information available (Wagener and Gupta, 2005). Parameter estimation in rainfall-runoff models is affected by uncertainties in the observed historical forcing (e.g. rainfall, evapotranspiration) and/or basin response (typically runoff) data and model inconsistencies. The data errors from various model inputs are likely to be propagated to the model outputs resulting in bias and misrepresentation. This leads to unreliable model results affecting the whole chain of water resources decision making. It should also be noted that even if a unique solution were to be obtained there will be uncertainty in the parameter quantities. This is due to propagation of uncertainty through the model and the objective function, resulting in a comparison of uncertain quantities. The result is uncertainty in the value of the objective function, and hence uncertainty in the optimal parameter set. The Heteroscedastic Maximum Likelihood Estimator (HMLE, Sorooshian and Dracup, 1980) objective attempts to address the issue of uncertainty in the inputs to the objective function. Due to the high variability of rainfall in both space and time it is likely that input errors are likely to persist into the near future. This is in

spite of advances in data collection and model construction (Kavetski et al., 2006; Beven, 2001). The errors in the observed response data usually impact the calibration of the model. Model calibration depends entirely on the accuracy of the reference observed data, whose accuracy is in many cases difficult to guarantee. This influences the resulting parameter sets and the uncertainties will be propagated into any other processes dependent on the model results, e.g. catchment yield estimations and model regional applications. It is important to note that the method chosen for parameter estimation (model parameterization) has an impact on the resulting parameter sets. The problem of parameter uncertainty is more acute in ungauged and/or poorly gauged basins where there are no reference historical observations to guide parameter estimation (Wagener and Wheater, 2006). As parameter estimation is very important in model calibration and application in water resources estimation, reduction of parameter uncertainty is therefore critical to improve confidence in the use of model results. One simple way of reducing parameter uncertainty (and indeed uncertainty in general) would be to design less complicated, parsimonious model structures with a small number of parameters (e.g. Young et al., 1996; Perrin et al., 2003) which can be concisely defined physically. However, caution needs to be exercised in choosing the number of processes to be represented as too simple a model structure may be impossible to use outside the range of conditions for which it was calibrated (Wheater, 2005). Another way to counter parameter uncertainty is to increase the amount of information available to identify the parameters, e.g. increasing the number of output variables (Gupta et al., 1998). The success of this approach is dependent on the ability of the model structure to handle this extra load (Wheater, 2005; Beven, 2001). On the other hand the improved use of information already available to improve parameter identifiability is another alternative. For instance, different periods can be used to identify different parameters. This represents a multi-objective calibration approach for estimating model parameter values and evaluating model structural deficiencies (Gupta et al., 1998; Madsen, 2000; Wagener et al., 2001). Another approach to reduce parameter uncertainty is the use of *a priori* parameter estimation methods (Ao et al., 2006; Koren et al., 2004). The major attraction of this approach is that it manages to avoid the uncertainties related to the observed input and output data and, regionalization methods and relationships (Kapangaziwiri, 2008). However, it may be subject to uncertainties related to the physical basin property data. The approach taken in this study is to estimate parameter uncertainties in relation to expected uncertainties (expressed by variability) in the measurement of physical basin characteristics. In general the uncertainty in the parameter estimation

process can be attributed to a variety of sources including (see for example Wagener and Gupta, 2005; Ao et al., 2006):

- ❖ The quantity and quality input of data: (discussed earlier)
- ❖ The structure of the model: (discussed earlier).
- ❖ The choice of initial parameter boundaries: Parameter ranges are chosen to constrain the parameter space during optimization so that all possible models (model structure and parameter set) are included. If the parameter ranges are too restricted, acceptable models may be erroneously rejected, whereas if they are too wide the parameter quantities may cease to be meaningful or result in unnecessary model runs (Beven, 2001).
- ❖ The choice of model performance and evaluation criteria: The issue of assessment criteria of models has been discussed extensively in the literature (see Nash and Sutcliffe, 1970; Freer et al., 1996; Gupta et al., 1998; Liden and Harlin, 2000). The choice of objective functions for model performance and the algorithms for optimization evaluation affect the resultant parameters. It is also true that parameter values can vary with the type of objective function used for optimization (Sefe and Boughton, 1982). In many cases when a single objective function is adopted multiple and equally acceptable parameter combinations are possible. This non-uniqueness of model parameterization, resulting in many parameter sets that are equally good according to the assessment criterion, is known as equifinality (Beven, 1993; 2001). This is a product of interactions of parameters within the model, making parameters a lot less identifiable. Interactions between and among parameters should, however, decrease with an increase in the parsimony of the model structure (Spear et al., 1994).

The close association between parameter uncertainty and equifinality has resulted in substantial consideration in the literature over the past decade where alternatives to the equifinality concept have been offered (e.g. Gupta et al., 1998; Thiemann et al., 2001; Vrugt et al., 2003a; 2003c). The alternatives advocate the finding of an optimal parameter set through the use of Pareto (e.g. Yapo et al., 1998) or Bayesian (Boyle et al., 2000) methods in global and multi-objective algorithm uncertainty estimation. While these attempts are noble, in practice model calibration still shows that more than one model (structure and parameter set), rather than just a single optimum, can be acceptable due to

uncertainty. The notion of an optimal parameter set is considered both unwise and unpalatable especially when considered against uncertain model forcing data, model structures and incomplete and limited process understanding (Beven, 2006). It seems indeed futile to expect imperfect representations to produce perfect results. The logical and practical approach in the meantime is to learn to live with the inherent uncertainties in modelling and assess how water resources decisions can be made in the presence of these uncertainties. In the long term, efforts to deal with the sources of uncertainties that can be reduced should be vigorously pursued.

It is a fact that uncertainty affects modelling results and their reliability and the confidence that can be expressed in them (Uhlenbrook et al., 2004; Siebert and Beven, 2009). In practical applications of modelling, uncertainty significantly limits the use of models for such purposes as parameter regionalization or making predictions beyond the gauged circumstances, such as generating land-use or climate change scenarios (Melching et al., 1990; Harlin & Kung, 1992; Seibert and Beven, 2009). Consequently, one of the major goals in environmental modelling has been the identification and quantification of sources of uncertainty in the modelling process. The total uncertainty in the model simulations, global model uncertainty, can only be comprehensively assessed if/when uncertainty propagation through the model manages to take into account all the possible sources. In practice, however, this may not be possible for various reasons, chief of which is the availability of the necessary data to adequately characterize and describe these uncertainties. The need to account for uncertainty in hydrological modelling is leading towards some sort of shift in the philosophy of model applications, from procedures that focus on the identification of a single best model towards procedures that seek to reduce the uncertainty in the predictions of all possible models using various types of ensemble methods. Wagener et al., (2006a) explain this as a move in hydrology from a philosophy of "optimization" towards one of model "consistency" which emphasizes the need to find models that are consistent with the behavior of the real world system. The necessity of making predictions in ungauged basins has given rise to a re-evaluation of the way in which water resources estimations can be carried out, especially in data poor areas. The current favoured route has been the production of model output ensembles of possible process descriptions for a basin rather than one hydrology time series as has hitherto been the norm. However, there is still a considerable part of the hydrology community that favours optimality.

It seems that the science of considering uncertainty in environmental modelling will be a topical issue into the foreseeable future. While the simulation of water resources is quite advanced, it still remains difficult in many cases to confidently announce results as accurate. It is safe to accept that modellers and model users may never be able to know if their model results are accurate (Hughes, pers comm.). Uncertainty analysis should thus allow scientists to express the extent of their confidence in model results. The intention is to make better decisions in water resources management, planning and development. The incorporation of uncertainty into the generation of hydrologic predictions should provide decision makers with information that allows them to incorporate risk in decision making and therefore mitigate some of the social, economic and environmental impacts of inappropriate operating rules (Heuvelink et al., 2007; Ajami et al., 2008). From a more social perspective, it is professionally more honest (and safer for the modeller!) to present results including an estimation of uncertainty (professional integrity). While incorporating uncertainty into estimation tools may not be the easiest (nor the most convenient) of tasks, the consequences of ignoring it may be worse. Ignoring uncertainty could lead to unjustified confidence in hydrological and water resources estimations and predictions and a lack of appreciation of the risks associated with decision making in uncertain situations. If the extent of uncertainty in predictions is not known, then there is no incentive to improve the science of making predictions through improving data collection, parameter estimation approaches and the model structures.

2.2.3 Modelling uncertainty and decision making

Decisions about the exploitation and management of environmental systems require information about environmental variables. This has placed hydrological models at the centre of water resources (and other environmental disciplines) management as an invaluable source of information which is used as a basis for management and policy formulation. However, in spite of a relatively long history of the development and use of models in policy making there is still poor integration between modelling and the decision process (Maier and Ascough II, 2006; Ajami et al., 2008). With the uncertainties related to the modelling process and the attendant risks related to the decisions based on model results, it is therefore necessary to explore the impact of modelling uncertainty on the decision making process.

Middlemis (2000) contends that there is "a perception among the end-users that model capabilities may have been 'over-sold', and that there is a lack of consistency in approaches, communication and understanding among and between modellers and water resources managers, often resulting in considerable uncertainty for decision making". While this statement does not dispute the importance of modelling in generating valuable information, it puts into perspective the precarious relationship between modelling and decision making. Thus, in the decision making process, an acknowledgement and estimation of uncertainty constitute significant steps for establishing the merits or utility of model-generated data as an input (Dovers et al., 2001; Brown, 2004; Hughes and Kapangaziwiri, 2009) and for judging the credibility of decisions that are informed by these data (Beven, 2000). This should allay fears of over-selling of model capacities and inflated confidence in model outputs.

Uncertainty is usually understood to be a critical constraint for the decision making process, and as such it has to be eliminated as much as possible. The major problem with uncertainty in decision making is that it refers to the situation in which there is not a unique and objective description of the system to be modelled. There is a need for scientists to determine clearly how uncertainty should be addressed and communicated for it to be effective as a decision making tool. Irrespective of the way this is done, uncertainty needs to be clearly captured in order to adequately indicate where gaps in knowledge and understanding are. When this happens, incorporation of uncertainty becomes an innovative way of scientifically analyzing and presenting available data and this is critical for decision making. Considering uncertainty also affords modellers a platform to try to find more robust solutions and avoid the problems with using a single optimum solution such as over- or under-designing which may have huge financial implications in engineering projects. It increases the confidence that can be expressed in the results of models and consequently the decisions based on them (Ajami et al., 2007). The chief aim of uncertainty analysis in terms of resource management is to improve decision-making under uncertainty, where one has to select the optimal action from a set of feasible alternatives (Wood and Rodríguez-Iturbe, 1975; Marin, 1986). From a scientific viewpoint, uncertainty analysis is the key to improving understanding. To complete the process it would be prudent to also include a sensitivity analysis to test the robustness of the dominant alternative with respect to uncertainties in the prior probability distributions and modelling process. Uncertainty analysis should therefore help achieve both

decision robustness and expected utility (Caselton and Luo, 1992; Reggiani et al., 2009).

Uncertainty analysis can be taken as a resource to determine the range of plausible scenarios and can aid the understanding of the process of change in a given system. Rather than being viewed negatively, the incorporation of uncertainty, given the understanding of the limitations of scientific expert knowledge, in decision making improves not only the credibility of science as a basis for decision making but also the decisions themselves. However, from a practical point of view, decision making is possible when model predictions are constrained within manageable bounds. It should also be emphasized here that there is a need for managers to think about how they should manage resources in the presence of uncertainty. The question that should be answered by both the scientific community and practitioners when it comes to decision making under uncertainty is, "how much uncertainty can the decision/policy maker handle"? Such an approach questions the utility of the uncertainty bounds that may be delivered to the decision maker. If the bounds are too wide, then there would be too much information, meaning that the uncertainty would have been over-estimated and it would be difficult for the decision maker to make any credible conclusions, while it may be equally difficult to utilise bands that are too narrow (Leamer, 1990). In the former case, decisions would tend to be conservative, while decisions based on the latter may tend to exceed their scientific credibility. Both have financial repercussions. Narrow bands around an observation may induce false confidence unless there is high confidence in the accuracy of the observation and/or the bands realistically represent the uncertainty. If the actual uncertainty is too wide to permit suitable decisions to be made, then it would be prudent to invest in better measurements and/or models. Leamer (1990) insists that the bands should "be narrow enough to be useful." This entails that, for a successful contribution of the modeller to decision making, there is need for communication between and among scientists and all stakeholders (Hughes et al., 2009). Science therefore has to balance between development of technical and formal methods to characterize and analyse uncertainty, and the communication with the stakeholders (in both bottom-up and top-down approaches) to determine the needs of decision makers (and improve relevance of their technical advancements, Maier and Ascough II, 2006). It is impossible for both groups to be highly knowledgeable about what the other does; decision/policy makers hardly understand models and modellers are not always conversant with the decision/policy process. Interaction is therefore important.

2.2.4 Estimating uncertainty

Uncertainties cannot be completely eliminated and, at best, they can be reduced by better equipment, improvements of standard data collection procedures, denser networks and maintenance. Uncertainty analysis is carried out to determine the statistical properties of the output as a function of input stochastic parameters (Lioy, 2009). This helps find the contribution of each input variable to the overall uncertainty of the model output and can be used to reduce the output uncertainty. From a practical point of view, uncertainty does not cease to be a problem once it has been reliably quantified but the problem has been significantly reduced. For instance, the problem of finding and using an optimal solution becomes redundant when one successfully quantifies the uncertainty related to any solution. It is therefore necessary that scientists be able to estimate uncertainty. Successful quantification, ensured through testing in gauged basins, would increase the confidence of making predictions in ungauged or poorly gauged basins (van der Sluijs et al., 2005; Refsgaard et al., 2007). In theory the estimation of uncertainty is quite simple. In the ideal situation one would use the full joint probability distribution function (PDF) of all sources of uncertainty and propagate this through the model to the model outputs. This would give the full picture of uncertainty related to the modelling exercise. However, in reality such a joint PDF is impossible to estimate because the interactions between the inputs are never completely known. Thus, in practice the best case scenario is usually that the statistical/frequency characteristics of some of the inputs and parameters are estimated. The choice of these variables is determined by availability of data and ease of estimation of the PDF. The later is usually the most difficult part for most environmental variables. Consequently, global uncertainty estimation (i.e. estimation of uncertainty for the model output) should be achieved using confidence bands/intervals, prediction intervals, inter-quartile ranges, variance (standard deviation) of or around the mean output (Montanari, 2004). Any representation of the form $(\mathbf{x} \pm \mathbf{y})$, where $\mathbf{x}$ is a mean value of output and $\mathbf{y}$ is a measure of uncertainty) is acceptable. If the confidence bands are wide (i.e. $\mathbf{y}$ is large), the output may not be a good approximation of the system behaviour, while it is a good estimate if the bands are narrow. In gauged basins, if the observed behaviour (assumed reasonably accurate) is not contained within the band of possible outputs, then the mean output is not a good estimate of system behaviour. While this is quite simple, the main question is how to achieve this estimation of uncertainty. There are two possible approaches to this problem – the conventional statistical approach or less formal methods (based on the principles of Bayesian statistics) dependant on largely subjective

probability treatment. Montanari (2007) emphasizes the point that "...when only a limited amount of information is available the expression of uncertainty in terms of probability is not possible" and argues that "...much human reasoning about hydrological systems is possibilistic rather than strictly probabilistic". This statement lends support to the use of less formal approaches to uncertainty analysis.

The formal statistical approach, usually referred to as the frequentist approach, is dependent on the use of formal statistical probability methods and testing (including hypotheses testing). The frequentist method essentially focuses on the expected frequency of occurrence of the observed data from hypothetical replicates of sampling. Caution ought to be exercised, however, as with any conventional statistical analysis, it works well and is reliable with long observed records but is unreliable and uncertain with short ones. This therefore makes it impossible to directly apply in ungauged basins. The implication is that its indirect use in ungauged basins entails dependence on any one of the many regionalisation approaches currently available. Given the heterogeneity of the land surface, this is unlikely to be a good approach. The frequentist approach is based on the classical Laplace probability which contends that the probability of an event is the ratio of the number of favourable cases, compared to the whole number of possible cases when nothing justifies an expectation of any one of these cases occurring more frequently than any of the others (Montanari and Brath, 2004; Montanari, 2004). Thus, from a hydrological modelling standpoint, if there exist sufficiently large data sets of historical observations, this approach would enable the inference of the uncertainty of these data premised on stationarity of the underlying processes. In the absence of such data, as is the case in many basins of the world, conventional frequentist statistics would lead to erroneous interpretations and conclusions.

The alternative that should work better for non-stationary physical hydrological processes and their deterministic modelling is a collection of less formal methods that are largely based on the fundamentals of Bayesian probability statistics. There has been growing tendency in hydrological modelling (especially in uncertainty estimation) to use these subjective methods due to the flexibility and subjectivity allowable with the approach. Typical examples of this approach are the use of fuzzy set theory and logic (e.g. Bardossy et al., 1990; Blazkova and Beven, 2002; Ozbek and Pinder, 2006), possibility theory (Cazemier et al., 2001; Mujumdar et al., 2009) and the Bayesian probability (e.g. Beven and Binley, 1992; Krzysztofowicz, 1999; 2001). In the Bayesian methods prior knowledge

and new data are combined using a model to produce posterior knowledge, or to update knowledge. The Bayesian inference provides a different but robust philosophical approach to uncertainty estimation. Typical Bayesian statistics interpret the concept of probability as the degree of belief in (i.e. uncertainty about) the occurrence of an event (Spiegelhalter and Rice, 2009). The most significant difference between Bayesian methods and their likelihood-based counterparts is the incorporation of prior information/knowledge (based on observations or experience) about system variables using prior probabilities. In practical application of the Bayesian methods the prior probabilities are weighted and combined in a model to estimate posterior probabilities. While conventional statistics are based on the probability of occurrence of the data "given that the various hypotheses are true" (McCarthy, 2007), the Bayesian approaches are based on interrogating the "probability of the hypotheses being true given the observed data" (McCarthy, 2007). While the use of prior knowledge is the strength and attraction of the Bayesian methods, the associated subjectivity has attracted criticism.

For uncertainty estimation in hydrological modelling, use of Bayesian approaches is less restrictive and more appealing; hence the popularity of such approaches such as the Generalised Least Squares Uncertainty Estimation (GLUE) of Beven and Binley (1992). While historical observations of stream flow usually constitute the prior knowledge for the conditioning of flow simulations, one of the questions that may be relevant is the extent of incompleteness of a gauged record that can be used for this purpose (Seibert and Beven, 2009). Can the Bayesian approach be used to accommodate very short (or few data points that may have been taken at irregular intervals) data periods or data with many missing values, by allowing for the large uncertainty within the prior knowledge? Where no or insufficient data are available some other knowledge can be used within the Bayesian methods to define prior knowledge, e.g. use of hydrological response characteristics (Shamir, et al., 2005, Yadav et al., 2007), catchment similarity indices (Wagener et al., 2007), regionalization based on limited gauges (Bulygina et al., 2009) or *a priori* parameter estimation (Duan et al., 2006; Koren et al., 2004). This presupposes the possibility of defining some formal probability distribution functions for these kinds of knowledge that can be used to constrain output uncertainties. One therefore supposes that an improvement in the knowledge should reduce predictive uncertainty. The approach taken in this study combines the use of *a priori* parameter estimation and regionalized indices of

hydrological response characteristics to constrain model output uncertainty (Kapangaziwiri et al., 2009).

The advantages of the Bayesian approach are that it provides a theoretically consistent way of thinking about statistical decision making, allows the explicit modelling of uncertainty in parameters and provides a theoretically consistent framework for integrating information from local at-site historical observations with regional hydrologic information and data from other sources. The Bayesian approach suggests that supplemental regional hydrologic information should be incorporated through a prior probability distribution to augment the information provided by the gauged record for a site (Vicens et al., 1975b; Kuzcera, 1982; Stedinger, 1983). Unfortunately, the actual updating or integrating step is straightforward for only a few simple distributions, and the use of prior distributions is sometimes controversial (Watson and Burnett, 1995).

Regardless of the approach adopted, most uncertainty estimation procedures are based on the following (Brugnach et al., 2008):

- ❖ Define how to measure the level of consistency between the simulated (Q_s) and observed (Q_o) system behavior

$$Q_o = Q_s + \varepsilon_o$$

where ε_o is usually a time series but needs to be reduced to a single number.

- ❖ Locate all (or a representative set of) models that comply with this definition in the feasible model space.
- ❖ Propagate the predictions of these models into the output space while considering other uncertainties

These steps try to answer the three aspects that need to be addressed in any attempt at uncertainty estimation, which are understanding, quantification and reduction of uncertainty (Liu and Gupta, 2007). The technical implementation of the steps has resulted in numerous frameworks and techniques in the past few decades (see section 2.2.4.1). One of the common factors of almost all the frameworks is that they perform detailed examinations of system conditions (learning from the model and/or data - Gupta et al., 2008; Beven, 2006; Beven and Freer, 2001) to gain adequate insight and understanding, which intelligence allows them to delegate credible probabilities (defining uncertainty) to possible

outcomes. The prominent basis of most of the frameworks are fairly common semi-analytic or numerical sampling based methods which work independent of model equations or even the model code. These methods generate a predetermined number of sets of inputs that are used to generate multiple outputs. A relationship is then established between the inputs and outputs using the model results at the sample points. The most common sampling based uncertainty analysis methods are the Monte Carlo and Latin Hypercube Sampling methods, Fourier Amplitude Sensitivity Test (FAST), reliability based methods and response surface methods.

Monte Carlo Sampling Methods: By far the most common methods for uncertainty analysis are based on Monte Carlo sampling, with a wide range of applications. Monte Carlo methods are based on random sampling from distributions of inputs and the use of multiple model runs to generate a distribution of output. They can thus be used to solve uncertainty propagation in models (Doll and Freeman, 1986; Fishman, 1996). In order to generate a reasonable distribution of the outputs, Monte Carlo simulations therefore require a large number of samples. This is a major weakness of the methods as time and resources needed to run the methods may be very high especially for some complex models. However, computational efficiency is usually achieved through some sort of modification of the methods that improves the sampling from the input distributions.

One such constraining technique is Latin Hypercube sampling, where the range of probable values for each uncertain input parameter is divided into segments of equal probability of occurrence and each parameter is sampled once from each of its possible segments (Stein, 1987). This results in random samples being generated from the full range of variability including extremes. The output will thus be more representative.

FAST (Fourier Amplitude Sensitivity Test, Saltelli et al., 1999): The FAST method is used to calculate the relative variance contribution of each uncertain input parameter to the total variance of model outputs. Basically, it is based on the consolidation, using Fourier transformation, of the uncertain inputs into a single frequency output (Saltelli and Bolado, 1998). Cumulative probability functions can be used to transform any other distributions that are not uniform for FAST and this reduces errors, improving the accuracy of transformation and making it more convenient in practical applications (Fang et al., 2003). Like SOBOL (Sobol, 1993), FAST does not need a linear or additive model behavior for

quantitative sensitivity and/or uncertainty analysis. The structure of the model to be analyzed does not have to be known. Notwithstanding the apparent versatility and, therefore, wider applicability of Monte Carlo methods, FAST has also been applied in many studies related to model sensitivity and/or uncertainty (e.g. Saltelli et al., 1999; Fang et al., 2003; Deflandre et al., 2005). The main advantages of the extended FAST are its robustness, especially at low sample size, and its computational efficacy (Saltelli et al., 1999).

Reliability Based Methods: FORM/SORM (First/Second Order Reliability Method, Cawfield, 2000): FORM and SORM are approximation methods that estimate the probability of an event (typically referred to as 'failure'). FORM and SORM are useful methods when the analyst is not interested in the magnitude of the model output, and its potential variation, but rather in the probability of the output exceeding some threshold value (Helton et al., 2006). FORM gives an estimate of how much a given input factor may drive the risk (probability of failure) of the system under study (Cawfield, 2000). SORM works in more or less the same manner as FORM serve for the fact that it involves a higher order approximation. This makes it more computationally demanding.

Response Surface Methods (Box and Wilson, 1951): These methods explore the relationships between several explanatory variables and one or more response variables. A response surface is a mathematical function that represents the behavior of a system, either real or simulated, by approximating the relationship between a set of its inputs and some given output variable (Fetel and Caumon, 2008). The methods consist of (i) screening to determine a subset of important model input parameters, (ii) making multiple runs of the computer model using specific values of these input parameters, and (iii) fitting a general polynomial model to the model data (using the method of least squares). This fitted response-surface is then used as a replacement (or proxy) for the computer model, and all inferences related to uncertainty analysis for the original model are derived from this fitted model (Box and Draper, 2007). These methods are an efficient approach for identifying statistically significant model parameters, and constructing response surfaces (Box and Draper, 2007). More recently, the surface response methods have been used to approximate the Pareto optimal front in multiple-objective optimization or calibration problems (Gupta et al., 1998; Vrugt et al., 2003a) in hydrological modelling (Yapo et al., 1998; Madsen, 2000) and have shown promise in their ability to provide useful insight into parameter uncertainty as well as model frailties (Gupta et al., 1998).

The other methods are the possibilistic (Montanari, 2007) and Bayesian methods (Neuman, 2003), explained before, and the inverse problem (Doherty and Johnston, 2003; Gallager and Doherty, 2007) and the fuzzy theory or worse case/best case scenarios (Kinzelbach, 2003).

2.2.5 Common contemporary technical approaches to uncertainty estimation in hydrological modelling

Several computer packages containing routines for many of the methods discussed above have been designed and are reported in the literature. The main aim of this section is to briefly discuss a small selection of the more common technical implementation tools/frameworks for uncertainty estimation and/or analysis that are currently being used in hydrological modelling. The major thrust in the examination of these techniques is in assessing their utility in areas/regions of data scarcity. The bulk of the materials that follows in this section has been paraphrased from the report on the PUB-IAHS Workshop on "Uncertainty Analysis in Environmental Modelling" held in July of 2004 where presentations were made on the various frameworks available for uncertainty analysis (www.es.lancs.ac.uk/hfdg/uncertainty_workshop/uncert_methods.htm). While some other literature sources were consulted, some sections or parts of the presentations have been adopted directly into this review.

GLUE (Generalised Likelihood Uncertainty Estimation, Beven and Binley, 1992): This is probably the most widely known and commonly used framework to investigate, quantify and analyse uncertainty of model simulations. It is the forerunner of the family of techniques that do not use conventional statistical approaches. The Generalised Likelihood Uncertainty Estimation (GLUE) methodology (Beven and Binley, 1992) was developed in an attempt to directly account for uncertainty in hydrological models. GLUE is designed to accept several different models that are consistent with observed response (i.e. behavioural) while those considered non-behavioural are rejected. This is achieved through the use of a likelihood criterion, which assigns zero likelihood to the non-behavioural models (Freer et al., 2003). The behavioural models can be statistically analysed to determine prediction boundaries, e.g. 95% prediction limits around the mean of the distribution of the behavioural outputs. A comparison of the observed response and the model outputs can reveal whether or not the observation falls within these boundaries.

The main underlying assumption of the GLUE framework is that the likelihood measure for each parameter is non-negative (non-zero for all behavioural models and zero for non-behavioural) and increases monotonically with increasing model performance (Beven and Binley, 1992; Beven and Freer, 2001). It also assumes stationarity of the error function between the calibration and validation periods.

The main strengths of GLUE are that the framework (Beven, 2006; Beven and Freer, 2001; Freer et al, 2003):

- ❖ Explicitly accounts for uncertainty in model structures and parameter sets, thus allowing for all possible valid models to be evaluated.
- ❖ Ability to incorporate new data to update prior knowledge about models or parameters
- ❖ Allows that behavioural models may be scattered throughout the parameter space.
- ❖ It is not model specific and can allow any model structure to be evaluated
- ❖ Can be used as a platform for learning from models (Gupta et al., 2008) especially in cases where more models are rejected than accepted.

The main weaknesses of the framework are;

- ❖ Subjectivity of the assumptions on which the framework is based especially the lack of formal assumptions in assessing the likelihood of different models (Mantovan and Todini, 2006).
- ❖ Inefficient sampling method: The framework uses uniform sampling in the parameter space which is not the most efficient even for simple response surfaces (Blasone et al., 2008). This results in high computational demands especially with complex and/or high dimensional models (Hossain and Anagnostou, 2005).

BATEA (Bayesian Total Error Analysis, Kuzcera et al., 2006; Kavetski et al., 2006): BATEA provides a platform for directly addressing of all sources of uncertainty in the calibration of conceptual type models (Thyer et al., 2007). It uses explicit probabilistic error models to estimate the uncertainty associated with observed input data (especially rainfall, Kavetski et al., 2006). The basic idea of BATEA is to represent the conceptual hydrological model and its error models as a Bayesian hierarchical model with additional variables describing errors in the data and the conceptual model. These additional variables filter out the input error given the model hypothesis and the observed data. It is based on the premise of an error model that is stationary over time (Kuzcera et al., 2006) and that the

input uncertainty is independent for each storm event though there is an allowance to use alternative uncertainty models.

The main advantages of BATEA can be summarized as (Thyer et al., 2007; Kavetski et al., 2006):

- ❖ Explicitly accounts for different sources of uncertainty. This allows for the separation, analysis of and learning from the different sources.
- ❖ Flexible in that it can handle the evaluation of alternative input and output error models.

The main weaknesses are:

- ❖ Computationally demanding.
- ❖ The need to specify valid error models, which are currently poorly understood.
- ❖ It relies heavily on the availability and accuracy of historical observations of stream discharge.
- ❖ Subjectivity on the assumed statistical inference which is conditioned on the conceptual and error models.
- ❖ The assumption of stationarity of the error model.

DYNIA (*Dynamic Identifiability Analysis*, Wagener et al, 2003): The DYNIA approach is used to locate periods of high identifiability for individual parameters and to objectively detect failures of model structures. It is based on the main tenets of the Regional Sensitivity Analysis (RSA, Hornberger and Spear, 1981), and GLUE (Beven and Binley, 1992) approaches. Basically, DYNIA divides a calibration time series into a sequence of small windows (time steps). For each window, it identifies parameter sets that allow the model to best reproduce the observations and then plots the distributions of the preferred parameter values as a function of time. The dotted plots are analysed to identify periods of high identifiability. If there are many local optima or near optimal values scattered throughout the response surface, it may be difficult to identify optimal parameter values (Wagener et al., 2004). DYNIA uses Monte Carlo to sample from an assumed uniform prior distribution of the feasible parameter space. If the parameter values change through time, it suggests that, within the model, the parameters are being adjusted to overcome shortcomings in the model structure (DeMaria et al., 2007). However, it must be remembered that using parameter variation as an indicator of model structural failures assumes time invariance of the catchment processes described by the parameter. Variation in values of the preferred parameter in those circumstances rather corroborates the model

structure and is not necessarily an indication of failure (Tripp and Niemann, 2008). This is however true only if this variation is correct.

The main strengths of DYNIA are summarized as follows (Wagener et al., 2003; 2004):

- ❖ Robust based on its ability to analyse parameter variation in time and identify and separate periods of noise from information. Its parameter estimation enables it to be used as a surrogate for model calibration.
- ❖ Model independent as it can be used with any structure and can also be used in an offline mode.
- ❖ Allows learning from the models and identification of possible uncertainties.
- ❖ Flexible with choice of model performance assessment criteria.

The disadvantages of the framework are;

- ❖ Determination of feasible parameter ranges may be subjective.
- ❖ Adequate representation of the shape of response surface requires a large number of models. That makes it computationally demanding.
- ❖ Poorly defined response surfaces, with near optimal parameters located far from the peak, are a problem. The proposed measure of identifiability will fail.
- ❖ Does not explicitly consider parameter interactions which are important in defining the shape of the response surface.

DBM (Data-Based Mechanistic modelling, Young and Beven, 1994; Young, 1998; 2001): The DBM approach is an example of the solution of the environmental modelling problem by having it posed as an inverse problem. The DBM modelling philosophy is based on the construction of 'parametrically efficient, low order, *dominant mode* models' (Young, 1998). In the DBM modelling approach, the model structure is first identified using objective methods of time series analysis based on a given general class of time series model (e.g. linear or continuous-time transfer functions). The resultant model is only acceptable if, in addition to adequately explaining the historical observations, it can be explained in physically meaningful terms. The initial model identification phase is essentially Bayesian in that it assumes that the parameters and inputs of the initial deterministic model are uncertain and can only be estimated using distribution functions (Young, 1999; 2001). The propagation of the uncertainty is achieved through a Monte Carlo simulation which also identifies the dominant modes model. The effects of uncertainty can therefore be evaluated efficiently given the

stochastic nature of the DBM model. The basic assumption in this approach is the existence of suitable observed data to generate the model structure, which makes it difficult to apply in data scarce regions of the world. If used in such regions then uncertainties are likely to be large, making it an unsuitable candidate to aid decision making.

The main strengths of the DBM approach are:

- ❖ The physical relevance of the model and the direct relation of the mathematical relationships to the scale of the time-series measurements used in their derivation (Young, 1999). This is important when making deductions from the modelling results.
- ❖ Versatility in that it can be used in a wide range of applications (e.g. forecasting) and can be used for both online and offline applications (Young, 2001).
- ❖ Its simplicity and ability to characterise the dominant modal behaviour of a dynamic system. This makes such a model an ideal basis for model-based control system design (Young and Chotai, 2001).

The weaknesses of the approach are related to its dependence on observations whose accuracy cannot be guaranteed. This implies that the quality of the data is paramount before a model can be developed.

PIMLI (*Parameter Identification Method based on the Localization of Information*, Vrugt et al., 2001): This is used to estimate model parameters and the approach is based on the Bayesian recursive estimation technique (BARE) of Thiemann et al. (2001) and the Generalised Sensitivity Analysis (GSA) of Spear and Hornberger (1980). The approach essentially advocates the existence of an optimum solution (i.e. parameter set). The observed record is subdivided into smaller datasets, each of whose impact on the sensitivity of the model to the parameters is evaluated (see also Wagener et al., 2003). PIMLI then uses the “variability in time of the model sensitivity for the various parameters to split the total set of measurements into disjunctive subsets that each contain the most information on one of the model parameters” (Vrugt et al., 2001). Each of the sub-datasets is then utilized for the constraining of its corresponding parameter. It assumes an invariable model structure and its inputs.

The strengths of the PIMLI method are (Vrugt et al., 2002; 2003b; Larsbo and Jarvis, 2006):

- ❖ Identification of a unique optimal parameter set.

- ❖ Enables direct uncertainty estimation through generating classical Bayesian uncertainty bounds on the model predictions.

The perceived weaknesses of the method are:

- ❖ Does not explicitly consider uncertainty in the parameter estimation, nor structure or input uncertainties which impact on parameter identifiability.
- ❖ High computational demands
- ❖ Depends on availability of observations whose quality cannot be guaranteed in many places.

SCEM –UA (Shuffled Complex Evolution Metropolis global optimization algorithm, Vrugt et al., 2003a):

The SCEM-UA global optimization algorithm is a Markov Chain Monte Carlo (MCMC) sampling algorithm used to infer the posterior probability distribution of model parameters. MCMC provides a solution to the difficult problem of sampling from a high dimensional distribution for the purpose of numerical integration. The idea behind MCMC for Bayesian inference is to create a random walk (called Markov process) and then to run the process long enough so that the resulting sample closely approximates the original population from which the sample was taken (Glimm and Sharp, 1999). These samples can be used directly for parameter inference and prediction. SCEM-UA uses complex shuffling to continuously update the prior distribution to a posterior distribution.

The reported advantages of the method are:

- ❖ Efficient in that it can generate explicit estimates of parameter uncertainty and prediction uncertainty bounds on the model outputs. .
- ❖ Comprehensive in its exploration of the whole feasible parameter range and also produces estimates of parameter sensitivity over this range.

The main weaknesses of the algorithm are:

- ❖ It is computationally demanding.
- ❖ Limited in its exploration of uncertainty as it ignores inputs and model structure uncertainty.

SODA (Simultaneous Optimisation and Data Assimilation, Vrugt et al., 2003c; 2005):

SODA, like BATEA (Kuzcera et al., 2006), tries to account for all sources of uncertainty, i.e. inputs, outputs and model structure. This is achieved through simultaneously applying parameter estimation optimization and data assimilation techniques using SCEM-UA (for efficient parameter exploration) and Ensemble Kalman Filter (for computational power and efficiency, Evensen, 2003).

For the estimation of the uncertainty associated with the output data, a non-parametric estimator is employed.

The main advantage of the method is (Vrugt et al., 2005):

- ❖ Comprehensive and accounts explicitly for all sources of uncertainty affecting hydrological modelling and produces uncertainty bounds on model simulations.

Unfortunately, given the complexity and extent of the uncertainties being considered, the method is computationally taxing. The method, like BATEA, can be model sensitive as they use the model outputs to identify the uncertainty in the input data.

Use of qualitative information (Soft Data, Seibert and MacDonnell, 2002):

This approach is premised on the understanding that hydrologists have more knowledge about a system than they eventually use for model calibration and that a deliberate incorporation of this knowledge whenever possible would improve model simulations. Seibert and MacDonnell (2002) call this knowledge (or intelligence) soft data that are usually non-numerical in nature.

The biggest problem with this approach is the level of subjectivity that can pervade the modeling process. While that may be the case, the incorporation of all available intelligence about a given system should be more reasonable than ignoring potentially crucial hydrological knowledge (Bergstrom, 1991; Uhlenbrook and Sieber, 2005). The other disadvantage is the fact that the soft data would normally be acquired through extensive field experiments or through experience gathered over long periods. It is unreasonable to assume that in largely ungauged regions resources would be available to embark on such data (or experience) gathering expeditions when measurement networks are shrinking (Oyebande, 2001; Hughes, 2004b; WWAP, 2009). Besides, getting sufficient understanding will take time and spatial heterogeneity would dictate that a lot more data collection would be required in huge basins. Surely, it would be cheaper (in both the short and long terms) to put up a measurement station. This approach depends on the availability of observations before the soft data can be used to constrain and reduce uncertainty in the model outputs. Soft data should be used, whenever and wherever possible, to augment any other method. It is good scientific practice to use all the available knowledge (qualitative or quantitative) to restrain predictive uncertainty. Soft data provides additional

criteria for parameter estimation through the use of hydrological knowledge and reasoning.

Ensemble predictions

Problems in hydrological modeling and uncertainty estimation are accentuated in ungauged or altered (e.g. land use) basins, because of the unavailability of sufficient historical observations of flow for parameter estimation through calibration. Of the many potential approaches the most promising has been based on the use of ensemble predictions. The basic tenet is that a range of possible models describing a given system by an ensemble of predictions is developed through sampling from the feasible parameter space and different criteria are used to separate the most likely sets from the unlikely ones (Beven and Binley, 1992; Freer et al., 1996; Beven and Freer, 2001). Ensemble approaches are used in both gauged and ungauged basins and have been seen to perform much better in the former case even with a very limited observed data set (Beven and Seibert, 2009). Of practical importance for the application of this approach in ungauged basins is the development of rejection criteria to distinguish between the acceptable (i.e. behavioural) from the non-behavioural models since observations are not available. McIntyre et al. (2005) proposed ensemble modelling and weighted averaging to establish the best estimate of flow at the ungauged basins. Local models are used to estimate parameters for some gauged 'donor' basins, which are then used to develop relationships with catchment descriptors. The established relationships are used to guide the definition of prior and posterior likelihoods (based on some measure of similarity) for 'candidate' models of ensemble predictions in the ungauged basins. McIntyre et al., (2005) concede that while the ensemble of candidate models does provide some indication of the range of uncertainty in the ungauged basin, blind testing in gauged basins revealed the inability of the ranges to capture the high flows. The main disadvantages with this method are that it depends on the availability of observed data to establish parameters and therefore suffers the same problems as any other regionalization process. The other problem is that the choice of similarity measures is subjective (in the same manner as the GLUE approach) and weighted averaging is not robust enough to accurately estimate flow. Besides, it is not a good approach to try and establish a single optimum flow series based on uncertain inputs.

The approach by Yadav et al. (2007) is also based on ensemble predictions but uses the ranges of expected catchment behavioural indices to constrain the ensembles of any model at ungauged sites. Different catchment hydrologic response characteristics are estimated and regionalized in a framework that allows the incorporation of the uncertainties related to the estimation process, resulting in ranges of possible streamflow behaviour that can be used in ungauged basins. This extrapolation of catchment behaviour has huge potential for conditioning hydrologic modelling in ungauged basins. The ensembles result from a sampling of the uniform distributions of the feasible parameter space and the model simulations compared with the regionalized indices of catchment behaviour. Those model outputs falling outside pre-determined prediction limits of the indices are rejected. Working with same data set used in the Yadav et al. (2007) study, Zhang et al., (2008) extended the catchment behaviour indices approach to enable the use of multi-objective optimization for the identification of model ensembles in ungauged basins.

In general the main advantages of the catchment behaviour indices approach ensemble predictions in ungauged basins are (Yadav et al., 2007):

- ❖ Model independent, implying consistency of results even when used across different model structures.
- ❖ Avoids the impacts of parameter calibration and/or model structural error.
- ❖ Enables learning from the process about the controls on watershed response behavior at the scale of interest, which could guide an improved approach to watershed classification.

Summary

While the technical frameworks considered in this discussion constitute only a small fraction of the whole population of techniques available, an examination of the literature reveals that the use of Bayesian approaches (both formal and informal derivatives) is quite popular. Another pertinent observation is that while these elaborate and mathematically sound frameworks have facilitated the understanding and quantifying of predictive uncertainty, few have gone beyond that to methods that address the critical aspect of reduction of uncertainty in an explicit and cohesive way (Ajami et al., 2007). This is of practical significance – what do we do with the uncertain results? A pervading and somewhat worrying thread that runs through almost all of these elegant techniques is their reliance on observations for definition and/or analysis of the posterior distribution or error functions of simulations to estimate uncertainty. This is quite understandable

given that they are developed in regions where substantial historical observations are available (circumstances influence the models/techniques that are developed, Brugnach et al., 2008). However, in places with reduced hydrological data (short data records), these methods may be difficult to apply, possibly leading to poor conditioning in the estimation of uncertainty. The resultant confidence bands would be hardly reliable. Thus, in typical ungauged regions like southern Africa a lot of adaptations (and often compromises) have to be made to use many of these techniques. While the definition of 'ungauged' has been universally accepted, in practice (from experience with model application in southern Africa and informal discussions with scientists in the developed world) it appears to mean different things in different places. Otherwise, how does one explain the inability of methodologies apparently designed to work even in ungauged basins to be difficult to use in some places. As has been pointed out earlier, the southern African region does not have sufficient quantities and quality of observed data to be able to efficiently use most of these techniques. It is rather sad though true that most of the ungauged basins of the world are in the regions that are most vulnerable to water crises and require the ability to confidently and reliably quantify their water resources for reliable decision and/or policy making. Therefore, the question of practicality is pertinent in the evaluation of the frameworks for use in ungauged basins. While some components of some frameworks have the potential to be useful in the region and indeed the use of ensemble predictions would reasonably work, a complete package is not available. This author contends that the development of these frameworks and the models they have been tested with in different environments (in all senses) affects the transferability (and utility) of these frameworks in a different environmental setting. It is therefore necessary that the southern Africa region either develops its own frameworks that would work with current water resources estimation tools or work with the international community to enable the current crop of frameworks to be adapted to suit prevailing conditions. The latter may necessitate the re-coding of existing frameworks. The current study follows the latter option and tries to quantify and reduce predictive uncertainty in both gauged and ungauged basins based on the ensemble prediction approach

2.3 Uncertainty estimation in water resources in southern Africa

The consideration, let alone incorporation, of uncertainty in water resources estimation and analysis tools in southern Africa have been non-existent or at best

slow. Thus, there have been relatively few contributions from South Africa on the subject (Hughes 2004b). It is rather surprising that this is so given the water problems in the region and the need for water based developments. Huge decisions have thus been made based on modelling results using limited databases of observations but without incorporation (or even cursory mention) of the extent of the uncertainties related to both the forcing data and the model results. In a revealing article commenting on the impact of floods on engineering design, Alexander (2002) wrote that, "in the design of structures vulnerable to destruction or damage by floods there are no hydrological design standards or codes of practice, other than for dam spillway design. International guidelines and experienced South African hydrologists and designers have stressed the need for engineering judgement in the application of hydrological analyses. However, if hydrologists cannot quantify their uncertainty, how can this uncertainty be accommodated in the civil engineering design?". This statement highlights the need to not only acknowledge that hydrological models produce uncertain information, but to quantify this uncertainty for informed decision making. Uncertainty in hydrological modelling therefore seems to be a relatively new development in the region. As such, there are many dangers linked to the introduction of this new science into existing tools. The most significant consideration, however, seems to be that whatever the methods adopted for uncertainty analysis they must be compatible with the existing tools. These existing tools, have been tried and tested in the region and have become part of the culture in water resources estimations. Practitioners are likely to be more flexible to add to their existing standard methods than to try something completely different. The rationale is that a lot of work has already been done based on these methods and any changes to methods have to be sufficiently justified as they will potentially undo large amounts of work, national databases and conventional wisdom (e.g. for South Africa the WR90 by Midgley et al., 1994 and the WR2005 by Bailey, 2009).

The introduction of modeling uncertainty (investigation, analysis and reduction) into water resources estimation tools has been slow in the region. Liden et al. (2001) considered uncertainty in their work on sediment modelling of the Odzi River in Zimbabwe and Mkwanaenzi and Pegram (2004) also introduced the idea in their design of a nowcasting system for the eThekweni Metro in South Africa. Using the Pitman (Pitman, 1973; Hughes et al., 2006) monthly rainfall-runoff conceptual model, Sawunyama and Hughes (2007) assessed the impact of rainfall data uncertainties on simulated flows in southern Africa. This study revealed that

there are significant changes in runoff simulations when different rainfall realizations (representing different levels of uncertainty) are used. This is significant given the shrinkage of rainfall gauging networks in the region and the fact that models (and consequently decision making) are heavily dependant on the ability to represent the spatial and temporal variations of rainfall patterns and distributions. Sawunyama (2009) also incorporated more sources of uncertainty (including input data, parameters and water-use data except model structure) to judge their relative impact on model results. The preliminary results suggested that, within the Pitman model, the parameters contributed the greatest uncertainty. This study thus tries to identify parameter sets that enable the model to realistically predict the behaviour of the natural systems in southern Africa while explicitly accounting for uncertainties in the parameters. The major aim is to be able to improve model application in ungauged basins of the region. Methods need to be developed to achieve this and a framework is proposed (Chapter 3) to systematically go through the process and ensure consistency. It is a fact that the Pitman model is quite heavily parameterized (Kapangaziwiri, 2008), implying that some of the current methodologies may be difficult to adopt as they are likely to be computationally demanding in order to achieve reliable model uncertainties (e.g. GLUE, Beven and Binley, 1992). Where there is a paucity of prior information on the distribution of the parameters and/or acceptable parameter ranges, more model runs are usually necessary to achieve better representation of the response surface and, consequently, the prediction uncertainty.

2.4 Summary and concluding remarks

- ❖ Hydrological models are employed as an aid to water resources management. These models are far from perfect and their results are therefore uncertain. To increase confidence in the model results used for decision making and to reduce the risks associated with these decisions, it is therefore imperative that hydrologists seek to investigate, quantify and reduce uncertainty in their model results. The most common sources of uncertainty are model input, structure and parameter errors.
- ❖ Uncertainty is an important component in decision and/or policy making. Any decision made has an associated risk (which can be measured in financial terms) and failing to account for uncertainty may magnify this risk. Any country that makes practical use of hydrological models cannot therefore ignore uncertainty.

- ❖ Representing uncertainty is simple in principle. A number of different methods are available to make uncertainty estimations. The methods can be based on conventional statistical approaches or on less formal methods using Bayesian statistics.
- ❖ The reliance of most of the elaborate methods on historical observations makes them unsuitable for use in data scarce or ungauged basins. While regionalization techniques can be explored for the possible extension of the results of these methods to ungauged basins, the availability and quality of the data for the establishment of relationships are a huge problem in southern Africa. There is therefore a need to develop more robust methods for use in such regions.
- ❖ There is rarely mention of what should be done when results are uncertain beyond the usual that more data needs to be collected. But what happens in the meantime? Many methods concentrate on the identification, quantification and/or analysis of prediction uncertainty, without offering a way forward. In the end, decisions will continue to be made in the same manner as before. That defeats the purpose of embarking on the science of uncertainty, and does little to justify the huge resources expended.
- ❖ In the absence of observations to condition models and estimate parameters, the *a priori* method is an alternative. However this depends on availability of data on the physical basin physical and hydro-climatic attributes.
- ❖ Preliminary analysis of uncertainty using the monthly Pitman model have identified parameter uncertainty as contributing the most to overall predictive uncertainty in southern Africa. This has to be investigated and the uncertainty reduced. There is a strong case for the analysis of the sensitivity of the various parameters so as to ascertain their individual contributions to the overall determination of behavioural models.

CHAPTER 3

A FRAMEWORK FOR MODEL APPLICATION IN SOUTHERN AFRICA

3.1 Introduction

It was highlighted in the last two chapters that while there has been muted acknowledgement of uncertainty and its impacts in water resources estimation, planning and management in the southern African region, there has not been any concerted efforts to incorporate this into modelling tools. One possible reason is a lack of will and commonality for the methods required for adequate address of this problem. Another reason could be the lack of assessment of the risks posed by using uncertain results. This chapter makes a contribution to the development of an uncertainty framework for model application that can be used in the region. A common platform for model uncertainty evaluation is important for reduction of risk associated with model-based decisions. One of the main objectives of the International Association of Hydrological Sciences (IAHS) initiative on Prediction in Ungauged Basins (PUB) is to develop science that enables the prediction of the hydrological behaviour of any ungauged basin (Sivapalan et al., 2003). In spite of the nobility of this endeavour, hydrologists are aware that they may never achieve accurate predictions. However what is emerging as important in this exercise is the importance of uncertainty. The treatment of uncertainty in the whole process is essential to the problem of understanding what is really involved with making predictions in an ungauged basin (Meixner et al., 2004). Firstly one needs to identify the potential sources of uncertainty and quantify the uncertainty before attempting to reduce it. The need to explicitly incorporate uncertainty is leading to a shift in the philosophy in making hydrological predictions from optimization to consistency. The former seeks to identify a single best model usually through calibration against some historical observation. However, given the errors and uncertainty associated with observations (when available), it is possible that a number of equally likely models can describe a given system. Consistency is therefore the acceptance of more than one model as a representative of the expected system hydrological behaviour (Wagener et al., 2006a). The accepted ensemble of predictions should encompass all possible observations (if being assessed against observed data) obtainable if the attendant uncertainties and errors were accounted for. Consistency is measured in terms of the expected catchment response based on hydrological understanding,

underlying modelling assumptions or historical observations. This is a possible explanation of equifinality (Beven and Binley, 1992), where the incorporation of uncertainty in making hydrological predictions necessitates the acceptance of more than just one model structure/parameter set combination to describe expected behaviour in any given basin, even if the basin is gauged.

The classical approach to the search for an appropriate model to represent a given system is largely driven by identification of a single model (structure and parameter set) that optimizes some set performance criteria. Such criteria are typically one or more numerical objective functions that calculate the aggregated distance between the observed and simulated variable of interest (Wagener et al., 2006a; Son and Sivapalan, 2007) or visual examinations to evaluate the model's ability to reproduce observations. Such approaches are more focused on deterministic simulation and, in the process, ignore uncertainties (parametric or otherwise) in the development of measures of model performance. Hydrological models are abstractions of the real world physical processes and are therefore unlikely to evaluate all plausible responses. Also, most of the observed data, especially in the southern African region, are residuals measured at the basin outlet and heavily impacted by unquantified or poorly quantified upstream activities. Therefore, it is possible that more than one model (structure and parameter set) can be acceptable as being consistent with regards to observations or underlying assumptions or expected response based on the physical makeup of the basin. While such a philosophy explicitly allows the incorporation of anticipated uncertainties, it is necessary to determine the extent of this consistency and acceptability. This recognises the need for an objective and consistent filtering criteria and if this can be achieved then, at least in theory, predictions can be achieved in any ungauged basin.

3.2 Approaches to making predictions in ungauged basins

Until recently, the most common approach to making continuous hydrologic predictions in ungauged basins has been the extrapolation of information on model parameters from gauged basins in a process commonly known as regionalization (Nathan and McMahon, 1990). The basic tenet in regionalization is that, if there exists a relationship between model parameters and basin properties which holds for a gauged basin then flow simulations can be achieved in an ungauged basin which has similar physical attributes. However, the transition from the identification of local models at gauged basins to the establishment of

relationships for regional models suitable for ungauged sites have some significant shortcomings related to the uncertainties associated with the local models and how these are affected by data errors and their own parameter uncertainties (Wagener et al., 2004; Wagener and Wheater, 2006). The lack of sufficient sets of observed data to condition the local model through calibration has been the inherent weakness of the regionalization process in data deficient areas making it difficult to develop credible and robust regression relationships. While concerted efforts are being made to classify catchments based on hydrological response and other similarities (Wagener et al., 2007), it would be futile if regional model applications will depend on the existence of observations. If such efforts are to be valuable contributions to making predictions in ungauged basins, it is suggested that consistency rather than optimization be the objective. The paucity of observed records in many places of the world, especially in Southern Africa, and the uncertainties related to available records precludes calibration. In that case it is sensible to embark on methodologies that are capable of producing all possible scenarios consistent with model assumptions and physical hydrological understanding.

An innovative alternative strategy that has been tested in a number of areas was proposed by Yadav et al. (2007). The strategy is based on the use of regionalized dynamic catchment response signatures to characterize hydrological behaviour. This regionalization of the signatures, rather than model parameters, is more sensible in that the data required are usually available and/or the signatures can be determined from physical basin attributes. This strategy is a component of the signatures-based, diagnostic process of model application and evaluation advocated by Gupta et al. (2008). The approach incorporates modelling uncertainty analysis and deviates from traditional practice in that it does not just use statistically based objective functions to measure model performance. The reasoning is that these traditional approaches ignore hydrological understanding regarding how the model represents the functional behaviour of a catchment. Model diagnostic approaches are necessary given that the crop of complex models being developed is inevitably fraught with greater interdependencies of model components, limiting the effectiveness of contemporary evaluation techniques. The detail and complexity of current environmental models and the need to effectively learn from, evaluate and possibly correct them (Gupta et al., 2008) necessitates the need for effective diagnostic approaches. Diagnostic approaches according to Gupta et al. (2008) "must help illuminate to what degree a realistic representation of the real world has (or has not) been achieved and (more

importantly) how the model should be improved". The process of model evaluation makes use of catchment signature indices of dynamic system behaviour to constrain and condition continuous flow simulations at gauged and ungauged sites (Figure 3.1). Wagener et al. (2007) and Yadav et al. (2007) define a signature as an index of the response behaviour of a catchment at a given time-scale, which is reflective of a catchment's functional behaviour and can be regionalised. Since these constraints arise out of the theoretical basis for hydrological modelling it should be possible to test them against observed data (Gupta et al., 2008). Depending on the model, a range of constraints could be used and common ones include yield-storage curves, flow duration curve gradients, runoff ratio (runoff/precipitation or P/Q), aridity indices (precipitation/evapotranspiration or P/PE) and measures of discharge timing (Shamir et al., 2005). Yadav et al. (2007) showed that such signatures can be regionalized very well since they derive directly from observed streamflow, rather than from a noisy calibration process as in the case of model parameters. If the regionalization process includes estimates of uncertainty, then these regional signatures can be used as constraints on the behaviour of local hydrological models (Figure 3.1).

The link between 'input-state-output data' and 'static basin data' represents the regionalization process in which regional signatures of catchment response behavior are used to constrain model outputs. This approach uses direct measures (from observed information) of the catchment behaviour to determine whether model outputs are 'acceptable' or behavioural and has been tested in some United Kingdom catchments by Yadav et al. (2007). The catchment indices are regionalized through the use of simple regression relationships with the confidence limits used to define the distribution of possible 'behaviours' for each index. For any given set of initial parameter values (defined either as equally likely values within a range, or as some type of distribution function), the model can be run for all possible parameter combinations to generate an ensemble of outputs. Predicted values of indices are then calculated from the model outputs and compared with the regional values to determine acceptable outputs from the output ensembles (Yadav et al., 2007 and Gupta et al., 2008). These regional signatures can thus be seen as regional priors on the expected catchment streamflow behavior. Additional information can be included if local priors on the model parameters are derived from static basin characteristics such as soil or topographic data. Local priors can also be used if there are some observed data. Such a framework therefore allows for the use of both local and regional priors

and for testing their relative value. In the process it is inevitable to get a better understanding of the system under evaluation which is an important part of making reliable predictions especially in ungauged basins.

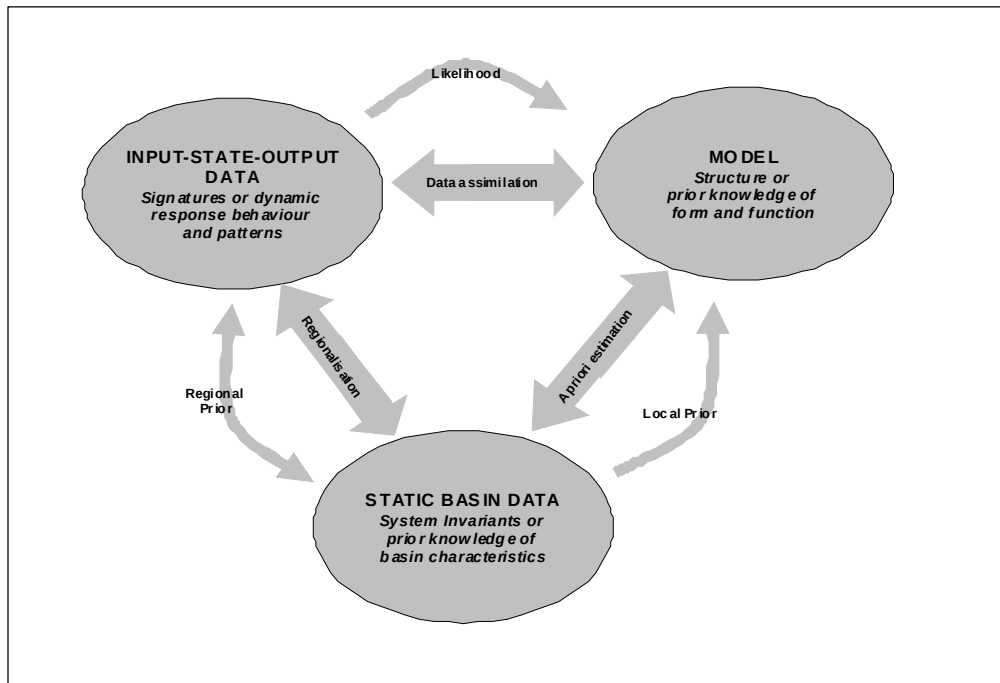


Figure 3.1 Diagrammatic representation of the use of priors in a model diagnostic approach used to constrain and evaluate model application (modified from Gupta et al., 2008)

3.3 A framework for model application in both gauged and ungauged basins.

While there has been general acknowledgement of uncertainty associated with water resources estimation in the southern African region (e.g. Ashton et al., 1999; Alexander, 2002), there has not been any concerted effort to research the sources of uncertainty nor its quantification and propagation through the estimation process. What is important is that the risks related to the use of uncertain model outputs be well understood or appreciated. The management of risk is essentially the ambit of decision makers and includes implementing risk reduction strategies, improving resilience to vulnerability and positioning resources to exploit opportunities (Mahomoud et al., 2009). The consideration and incorporation of uncertainty in water resources estimation would surely go a

long way in assisting water managers make more informed decisions. Model outcomes and the decisions based on them are left vulnerable if the uncertainties associated with the modelling process are not analysed and documented (Beven, 2000). Uncertainty assessment is increasingly being applied in water resources estimations and techniques used are varied and numerous. There are first-order uncertainty analysis methods (Melching et al., 1990), sensitivity analysis (Morris, 1991; Freer et al., 1996), Monte Carlo analysis (Seibert, 1997; Wagener et al., 2003), Bayesian uncertainty (Tol and de Vos, 1998), parameter uncertainty investigation by validation, or by uncertainty frameworks (the Generalised Least Squares Uncertainty Estimation, GLUE, Beven and Binley, 1992), Bayesian methods (Thiemann et al., 2001; Ajami et al., 2007) and Pareto Optimal Set procedures (Chankong and Haimes, 1993). Though all these approaches are commendable and can be used to achieve the objectives of quantification of uncertainty, identification of factors most influential to model predictions and generation of output most relevant to decision making, there is need for consistency of methodologies. What this implies is that there is need to identify an approach that is consistent with the practical requirements of water resources estimations, the types of models being used and the data available in any given region. In southern Africa, it is therefore prudent to have a framework for model application that;

- ❖ Is consistent (in terms of reproducibility and being in line with resources availability and modelling purpose) and explicitly includes uncertainty analysis in the generation of model outputs.
- ❖ Simple and robust in principle but flexible enough to be useable with any model structure.
- ❖ Can be applied with existing information or with information that is easily obtainable within the region.
- ❖ Provides a platform for model diagnostic evaluation.

A Water Research Commission (WRC) funded project on uncertainty in which the author is involved held a workshop in Pretoria during November 2008 to introduce the project to a range of stakeholders involved in water resources assessments or water resources decision making, as well as to define some of the technical approaches to the project in more detail. The main outcome of the workshop was the design of a consistent approach for including uncertainty analysis in the generation of hydrological model outputs that is independent of model type. Figure 3.2 illustrates the framework that has been adopted for use in southern

Africa with the support of the professionals that attended the workshop. The main components of the framework are the estimation of model parameters and definition of their distributions (Chapter 4), selection of a model structure and a sampling procedure to generate ensembles of simulations and the construction and application of model output constraints (Chapter 5).

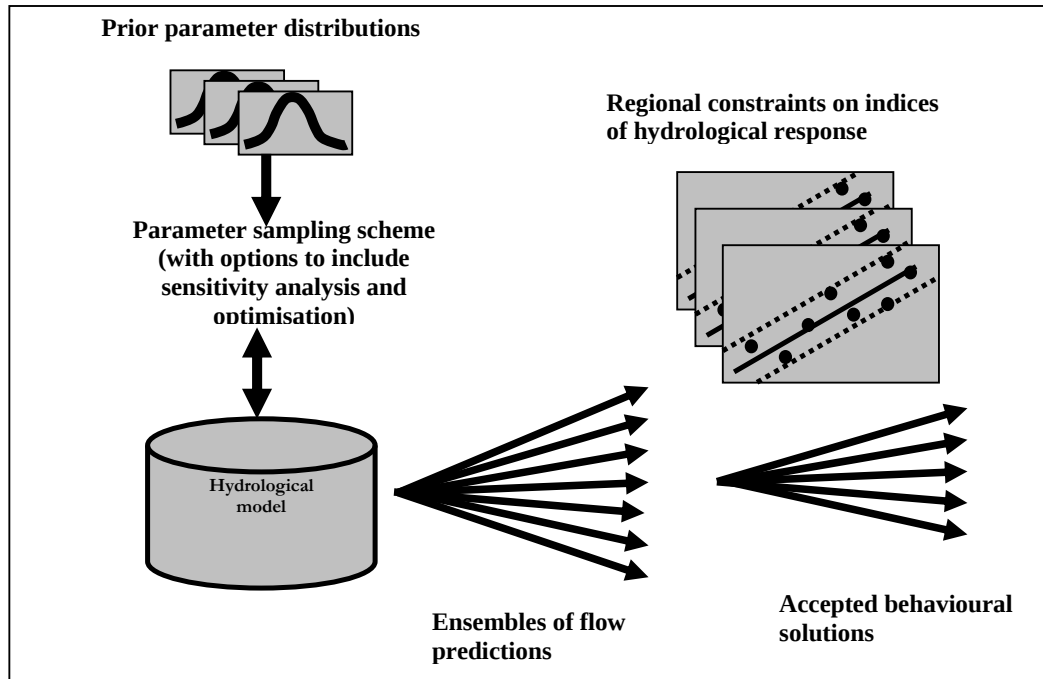


Figure 3.2 The model independent model application and evaluation framework that can be used in southern Africa

While the main components are discussed in later chapters, the basic concepts of the framework are outlined below. The starting point is to establish the prior uncertainty distributions of the parameters of the chosen model (Wagener and Wheeler, 2006; McCarthy, 2007; Munoz-Carpena et al., 2007). The approaches used to achieve this will inevitably be model dependent and may also vary from region to region for the same model. The nature of the distributions could also vary between models and between parameters. Some could be 'structured' distributions such as normal or log-normal distributions where reasonable information is available to suggest which parameter values are more probable than others. Other distributions could be 'unstructured' such as a uniform distribution defined simply by the specification of minimum and maximum values. In this case inadequate or no information exists to inform the likelihood estimates

of parameter values. The prior parameter distributions are used to generate multiple (say 10 000) parameter sets based on independent Monte Carlo sampling. It should be noted that overall results from Monte Carlo-based probabilistic assessments will always be influenced by the selection of input parameters to be included in the analysis (Nofziger et al., 1994), the type and parameterisation of probability distribution functions attributed to input parameters (Brattin et al., 1996), the absence/presence of correlation between variables, the extent of the correlations considered, the sampling scheme used (Saltelli et al., 2000) and the seed number used in the sampling (Dubus and Janssen, 2003). Running the model with all the parameter sets generates an equivalent number of output ensembles of flow predictions. It should be noted that not all of these ensembles will necessarily be consistent (i.e. behavioural, Beven, 2006) with expected hydrological behaviour. The filtering necessary to identify which of the model ensembles are behavioural is achieved by the use of constraints defined by the number of regionalized indices of hydrological behaviour. These indices, similar to the approach used by Yadav et al. (2007), are developed from observed hydrological responses and basin attributes. Such indices are expected to cover the range of hydrological regime characteristics (magnitude, frequency and duration) and some could either be shared by different models, or be specific to certain model types (i.e. indices based on daily flow regime variations would be relevant to daily models only). The use of indices is significant since they can provide insight into the functions of a catchment and are solid basis for a hydrologically relevant assessment for catchments. This is especially so when observed data are unavailable or insufficient. The regional constraints will also be subject to uncertainty, in that they are expected to be developed from imperfect relationships between observed indices of hydrological behaviour and prediction variables (for example, basin physical attributes) whose measurements are capable of being taken at all locations including ungauged sites. Thus, cognizance of this ought to be taken when the relationships are used to constrain the model outputs.

The formulation of the parameter distributions and the sampling scheme should be independent of the regional constraints. The parameter sampling scheme may be unconstrained by any prior knowledge (either because that intelligence doesn't exist or is not reasonably adequate), resulting in larger uncertainty than the regional constraint (Figure 3.3 A). On the other hand, the sampling scheme could be based on some parameter estimation process that already incorporates prior knowledge. In this case it is possible that this knowledge is better than the

knowledge contained within the regional constraints. This would give lower uncertainty in relation to the constraints (Figure 3.3 B).

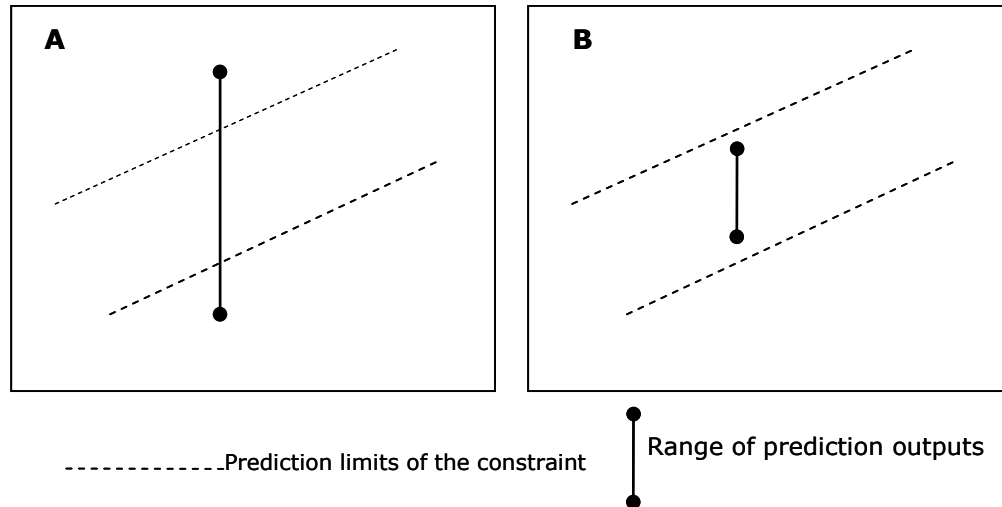


Figure 3.3 Illustration of the likely results of using prior knowledge to constrain parameter sampling scheme (B). Diagram A shows the result when little or no knowledge is used.

The Pitman model (Pitman, 1973) has enjoyed popular use in the region for a very long time and has become a standard water resources estimation tool. For this study, a revised semi-distributed version of the model that incorporates surface and ground water interactions (Hughes, 2004a; Hughes et al., 2006) is used to evaluate the use of the framework. Figure 3.4 is a flow diagram of the version of the Pitman model used in this study. The Pitman model is a monthly rainfall-runoff model whose inputs are monthly time series of rainfall totals and long term estimates of annual potential evapotranspiration. Though the model works on a monthly time scale the monthly rainfall totals are disaggregated into the four internal iterations over which the model works. The Pitman model is much like any typical conceptual model with tank type storages. Interception, soil moisture, and ground water are the three conceptual storages in the model. It also has routines to simulate human influences such as abstractions and impoundments. The current version of the Pitman model with ground water routines is quite heavily parameterized with a total of 41 parameters. The rationale is that the parameters “should be easier to evaluate for ungauged (or altered) situations because they are more meaningful in terms of real hydrological processes and can be related to measurable catchment characteristics” (Hughes,

2004a). However, most of the parameters can be estimated a priori from basin properties leaving some 11 free (calibration) parameters. The current study focuses on the development of uncertainty estimation procedures for these calibration parameters. Table 3.1 and Table 3.2 list the parameters of the model, including some brief explanations.

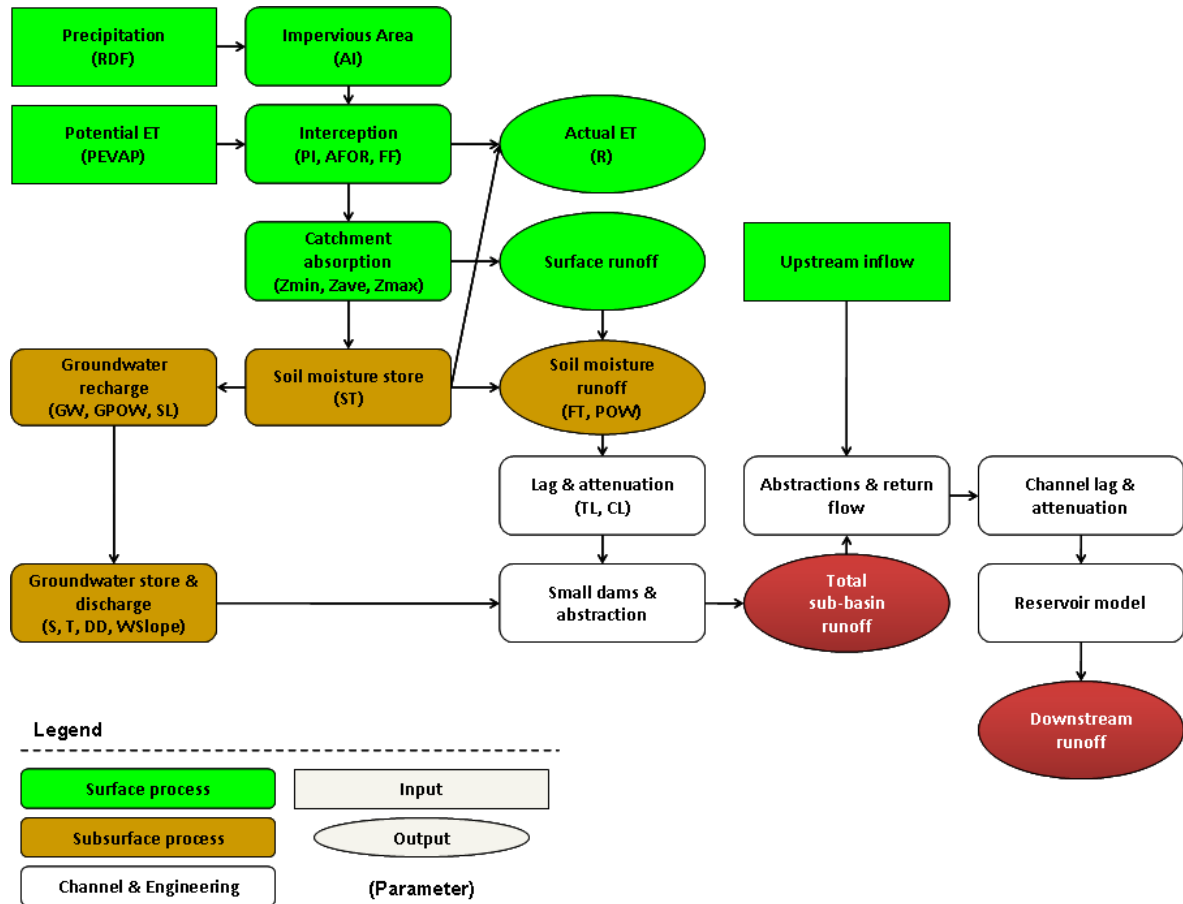


Figure 3.4 The flow diagram of the Pitman model showing the main model components and their relevant parameters.

Table 3.1 Parameters of surface process descriptions of the Pitman model

Parameter name	Units	Description of parameter
RDF	-	Rainfall Distribution Factor – influences the evenness of rainfall distribution into the four iterations of the model.
AI	%	Percentage of the area covered by impervious area which is contiguous to the river channel
PI	mm	Interception capacity of the vegetation in the basin. This parameter is specified for 2 dominant vegetation types for both summer and winter seasons.
AFOR	%	Percentage area of sub-basin under the second vegetation type
FF	-	Ratio of potential evaporation rate for vegetation type 2 relative to vegetation type 1
R	-	Evaporation-moisture storage relationship parameter
ZMIN	mm/month	Minimum sub-basin absorption rate
ZAVE	mm/month	Mean sub-basin absorption rate
ZMAX	mm/month	Maximum sub-basin absorption rate
TL	months	Lag of surface and soil moisture runoff
CL	months	Channel routing coefficient

Table 3.2 Parameters of sub-surface process descriptions of the Pitman model

Parameter name	Units	Description of parameter
ST	mm	Maximum moisture storage capacity
FT	mm/month	Runoff from moisture storage at full capacity (ST)
POW	-	Power of the moisture storage- runoff equation
SL	mm	Minimum moisture storage below which no GW recharge occurs
GW	mm/month	Maximum ground water recharge at full capacity, ST
GPOW	-	Power of the moisture storage-GW recharge equation
S	-	Ground water storativity
T	$\text{m}^2 \text{d}^{-1}$	Ground water transmissivity
DDENS	km km^{-2}	Drainage density
GWSlope	%	Initial regional ground water gradient for ground water movement

While this study only concentrates on parameter uncertainty, the framework can be used to assess any source of uncertainty including, but not limited to, model input data errors (e.g. rainfall, evaporation), model structure uncertainties and climate change scenarios and uncertainties. Figure 3.5 illustrates the flow diagram of the use of the framework with the Pitman model. This illustrates the options available in different circumstances. The parameter priors are estimated from basin property data and if not available attempts (not yet done) will be to use global datasets of remotely sensed data. If there are historical observed flow data, then the model outputs can be assessed against these through use of pre-determined objective functions. This conditions the local model. The observed

data could also be used in conjunction with basin attributes data to develop indices of dynamic catchment hydrological behaviour. In the absence of observed records of flow, the model outputs are assessed using regional hydrological signatures.

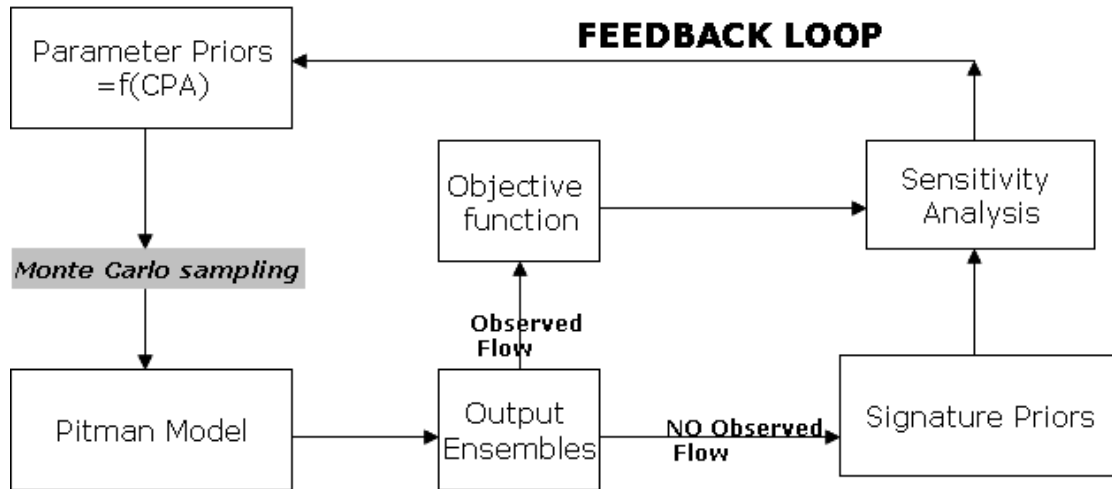


Figure 3.5 Flow diagram of the application of the Pitman monthly rainfall runoff model within the framework

For the assessment of parameter uncertainty two additions to the framework (Figure 3.2) were made. The first one relates to the sensitivity analysis. This is necessary in order to determine the parameters that have the most influence on the model simulations based on either the constraints or a statistical objective function (in the case of gauged catchments). The incorporation of sensitivity analysis into the framework is a way to assess the robustness of both the framework and the model in taking advantage of the knowledge of the watershed topography and physical make-up. After determining the regions of behavioural parameters, it is envisaged that optimization for the parameters can be done (Figure 3.2). For purposes of staying within the physically realistic ranges, the boundaries of such optimization would be defined by the uncertainty limits of the hydrological signatures. While the Pitman model has generally rarely been used in an optimization framework (Ndiritu, 2009; Ndiritu and Daniell, 2001), and optimization is generally used in gauged basin using observed data it is possible that the hydrological indices can be used to constrain the optimization of the model outputs within acceptable (i.e. behavioural) ranges. Depending on the results of this analysis it may be necessary to improve the intelligence used to constrain the estimation process of the parameter priors. This necessitates a

feedback loop to the prior parameters where adjustments can be carried out on the estimation equations. For instance, one can interrogate the parameters (or group of parameters) related to the non-behavioural ensembles to determine any common possible problems. The parameter estimation equations and/or the input physical data may then be reviewed accordingly.

3.4 Summary

The main conclusions that can be drawn from this chapter are:

- ❖ Many regionalization techniques have failed to provide adequate predictions in ungauged basins. Limited records to provide a critical mass for the development of regional relationships between parameter and basin attributes have made it difficult to use regionalization techniques in southern Africa.
- ❖ There is need to consider uncertainty in water resources management to improve the quality of model-based decisions. To achieve this, it is imperative to develop an uncertainty framework. Such a framework was presented in this chapter with components to estimate priors for parameters and constraints.
- ❖ This framework accounts for the various constraints expected to exist in the region related to, *inter alia*, data availability and accuracy, model preferences, capacity or willingness of practitioners to adopt new methods and access to specialized software.
- ❖ The framework can be used with and model structure and is capable of being used in both gauged and ungauged basins.
- ❖ The constraints provide a useful control on the model simulations especially in the ungauged basins. In the gauged basin these can be used to assess the reliability of both the model and the historical observations.
- ❖ The constraints are also subject to uncertainty, depending on the veracity of the data used to develop the constraints (Kennard et al., 2009). Variation in bias, precision and overall accuracy of these metrics influences the ability to correctly describe flow regimes and detect meaningful differences in hydrologic characteristics through time and space. The range of this uncertainty should be greater than that related to the model outputs for acceptable models.

A feedback loop is necessary in the framework in order to improve the parameter and uncertainty estimation processes. Model performance is assessed through the

use of signatures of hydrological behaviour in both the gauged and ungauged basins. The uncertainty constraints provide the physical boundaries of the hydrological process.

CHAPTER 4

PARAMETER PRIORS

4.1 Introduction

Hydrological predictions have been achieved through the use of various types of models, from simple lumped, through conceptual, to more complex distributed physically-based structures. A typical hydrological model consists of a large number of coupled equations describing the different natural hydrological processes. Thus, in spite of the complexity of the structures, nearly all models have parameters (some mere mathematical coefficients and others with physical significance) that must somehow be quantified. Clarke (1973) defines a parameter as a quantity that characterizes an aspect of a hydrological system in a particular basin and should remain constant in time. Parameters are basin or sub-basin specific with some expected to vary seasonally, and still others being dependent on the spatial or temporal scales used. For practical purposes to solve engineering problems, hydrologists and water resource managers have traditionally relied on "optimal" parameter estimates whose optimality is based on their sampling properties in the parameter space (e.g. mean square error, unbiasedness). A common example is the use of the maximum likelihood technique that has enjoyed popular use in both flood frequency studies and hydrological models. Marin (1986) argues that such measures may be inappropriate within the small sample size environment and the management, rather than inferential, focus of water resources planning. Given the many and varied sources of uncertainty characteristic of water resources planning, it is thus prudent to recognise that optimal parameters will not necessarily lead to optimal actions in the decision space.

The most common approach to the quantification of model parameters has been calibration where the parameters are adjusted until the simulation matches the observed measurements as closely as can be achieved. However, the information which is normally available for calibration (and validation), i.e. time series of driving variables and discharge, often does not allow a decision about which parameter set is the correct or optimal one (Sorooshian and Gupta, 1983). Model structural inconsistencies and errors in observed data, considered together with the more or less arbitrary choice of the objective functions makes it unreasonable to expect that any one parameter set will be optimal (Beven and Binley 1992).

From a set of ten objective functions, Sefe and Boughton (1982) concluded that parameter values varied with the type of objective function used for the optimization. Kuczera and Williams (1992) demonstrated that parameter uncertainty increases when errors in the areal rainfall used in the calibration period are considered. It can thus be concluded that parameter uncertainty can arise from many aspects of the modelling exercise. Therefore, given the pervasive uncertainties that characterise water resources estimation procedures, it is not too difficult to see that optimal parameters may not necessarily lead to optimal actions in the decision space.

The literature abounds with arguments for the use of other more statistical techniques (e.g. Bayesian procedures) for the estimation of model parameters in the water resource estimation problem (e.g. Thiemann et al., 2001; Beven and Binley, 1992; Kuczera and Parent, 1998) which incorporate the expected parameter uncertainties. The major impetus for the approach was given by Vicens et al. (1975a) who showed that incorporating parameter uncertainty resulted not only in different reservoir storage requirements but also led to more efficient decisions (reservoir size) than with maximum likelihood estimators (Marin, 1986). Such studies show the importance of parameter uncertainty in the overall modelling process, as opposed to some schools of thought that regard it as being only important for the simulations of the internal states and fluxes of the model. Parameter uncertainty does contribute significantly to the combined modelling uncertainty (Melching et al., 1990) and by including uncertainty in model parameters (and therefore model outputs) through the use of probability distribution functions (PDF), rather than using single estimates, it is envisaged that more information is available to the water resources managers with respect to prediction error. Uncertainty associated with model output may be represented as a probability distribution or as a specific statistical quantity, such as the 95th percentile from the cumulative probability distribution (i.e. what is the streamflow prediction that is equaled or exceeded 95% of the time?). By introducing notions of confidence and probability, this approach provides more information than a single estimate and informs policy developers about the degree of risk associated with particular actions (Benke et al., 2008).

This chapter therefore aims at providing answers to two fundamental questions in relation to the application of the Pitman rainfall-runoff model, which is popularly used in the region:

- ❖ How can the physical basin characteristics, and the role they play in the rainfall-runoff transfer processes, be used to directly (*a priori*) estimate hydrologically relevant parameters that can be used for large scale modelling in ungauged basins?
- ❖ How can the uncertainties associated with the physical basin property data used for the *a priori* estimation of the Pitman model parameters (Kapangaziwiri and Hughes, 2008) be accounted for?

Any attempts at answering these two questions can be presented in several different ways. Some ways would follow a top-down approach where the estimation of the parameters is discussed before the inclusion of uncertainty is tackled. The other is some type of bottom-up approach which starts with establishing the source of uncertainty and the data required to do the analysis and ends with the parameter estimation equations. In this study the former approach is deemed appropriate as it builds on the author's Master of Science (MSc) work where estimation procedures for most of the calibration parameters were established (Kapangaziwiri, 2008; Kapangaziwiri and Hughes, 2008). The next sub-section will give a synopsis of the principles, motivation and the equations of the *a priori* parameter estimation process. The derivation of the estimation equations, and the explanations thereof, for those parameters that were not part of the previous work (Kapangaziwiri, 2008) will be given in detail at the time of their discussion in section 4.2.

4.1.1 The parameter estimation approach

This main thrust of this part of the study is to explore the incorporation of uncertainty (section 4.2) into existing *a priori* parameter estimation approaches (Kapangaziwiri and Hughes, 2008; Kapangaziwiri, 2008). The parameter estimation procedures are motivated by the understanding that if parameter estimation could be achieved directly using physical basin attributes and the role that they play in the rainfall-runoff process, then it would lead to a more consistent approach to making hydrological predictions especially in the ungauged basins of the region. What these procedures entail is that the parameters should be hydrologically (and physically) relevant and have explicit conceptual physical meanings to enable the isolation of their individual effects. Such parameters would therefore help describe specific basin processes rather than multiple processes as is the case in many conceptual type applications. If that can be achieved then the need for basin-specific model calibration would be minimized,

leading to more consistent and objective results that can inform understanding about potential sources of uncertainty and how it is propagated into model simulations. Thus, such an approach provides a solid platform for the analysis of both predictive and parameter uncertainty with the aim of eventually reducing it (Kapangaziwiri, 2008).

The earlier work concluded that the *a priori* estimates of the soil moisture store (ST, uncertainty incorporation in section 4.2.1), runoff (FT, POW, uncertainty incorporation in section 4.2.2 and 4.2.3 respectively), and infiltration parameters (ZMIN, ZAVE, ZMAX, uncertainty incorporation in section 4.2.4) were quite successfully physically defined. Additional parameters estimated in this study are related to the evapotranspiration, groundwater recharge and interception processes. Given the model structure, it was reasonable to assume that the maximum soil moisture storage capacity parameter (ST) would represent both the storage in the soil layer and in the unsaturated fracture zone between the soil and the water table. The amount of moisture held in the soil component would depend on the soil's porosity and its depth, while the unsaturated zone capacity would be influenced by the storativity and depth of the fractured zone. This means that deep, well-drained soils and gentle slopes would hold more water (higher ST), while shallower soils, often more characteristic of steeper headwater basins, have lower ST values. The release (rate and magnitude) of the water from these storage components as interflow (maximum of FT mm month⁻¹) depends on the extent of topographic dissection (drainage density) and gradient, hydraulic conductivity, as well as the ability of the underlying geology to transmit the moisture from the unsaturated zone through fractures. Variations of interflow with the level of sub-basin storage (determined by parameter POW) is expected to vary with the spatial distribution of soil moisture storage which is influenced by basin slope and soil drainage characteristics that affect the rates and patterns of moisture re-distribution following storm events. POW defines the power (exponent) of the non-linear relationship between the soil moisture content and interflow. The basis for the estimation procedure for this parameter is the partial and variable source area concepts where the low-lying areas, rather than steeper areas, stay wetter and contribute interflow for longer. Within a basin, moisture movement is slower through poorly drained soils and gentle slopes (giving higher values of POW), but quite fast in steeper areas with well-drained soils (lower POW).

Parameters ZMIN, ZAVE and ZMAX are used to quantify the infiltration excess flow process in the model and therefore depend on the soil surface conditions (determining infiltration rates), the size of the soil moisture store, number and spacing of rain days (which influence the antecedent moisture conditions at the start of a rainstorm event) and typical storm durations (indicative of expected rainfall intensities).

The relationships between the physical basin attributes and the parameters were developed based on well understood physical hydrology principles. This approach results in the estimation of the best estimate (mean) parameter values based on physical basin attribute data that are likely to be available (albeit differing in detail and quality) in most countries in the region. The earlier work (Kapangaziwiri, 2008; Kapangaziwiri and Hughes, 2008) demonstrated that the physical estimation equations generally resulted in sensible parameter values and adequate simulations of hydrology compared with observed data. However, there were also situations where less than satisfactory simulations were achieved using single (mean) estimates of the parameter values, demonstrating that uncertainty exists in the use of the estimation equations. At least part of the uncertainty is associated with the subjectivity inherent in the interpretation of the physical basin property data. For example, soil depth and slope values are typically given as a range from which a representative value would be inferred. There is a potential for inconsistency in the estimation process because different users may infer different representative values for the same basin using the same data. The estimation process is particularly prone to inconsistency when there are a number of different soil units (each with ranges of depth and slope) within the sub-basin being modelled and from which a single representative value has to be estimated.

In an analysis of the contributions of different sources of uncertainty in the Pitman model, Sawunyama (2009) came to the conclusion that parameter uncertainty made the largest contribution to the uncertainty of model simulations. Hughes et al. (2010) investigated the propagation of parameter uncertainty by varying combinations of estimates of best parameter values based on their effect on flow generation (i.e. whether a combination produces higher or lower runoff) and concluded that a more robust analysis methodology needs to be developed for the application of the Pitman model in the region. The method used by Hughes et al. (2008; 2010) was discrete and did not explore the parameter space efficiently despite including all possible extreme parameter combinations. A parameter estimation process that directly incorporates measures of uncertainty

is therefore an imperative. The method presented here is based on the use of the range of variability in the input basin characteristics data to define the uncertainty in these data that will be propagated into the final values of the parameters. To do this efficiently requires a definition of the frequency or probability distribution functions (PDFs). If such PDFs are defined it then becomes a relatively straightforward task to generate samples (say 5000) from these distributions and run them through the parameter estimation equations. The results can then be used to define posterior PDFs of the estimated parameters that represent all the possible parameter values based on the variability of the physical property data. This approach has been adopted in this study and Section 4.2 gives full details of how the incorporation of uncertainty into the *a priori* parameter estimation procedures is achieved.

In the case of South Africa, the source of the majority of the information on the physical basin characteristics data is the Agricultural Geo-referenced Information System (AGIS, 2007) database described in the next subsection. While this database may not be as comprehensive as would have been desirable for the parameter estimation processes, it is the most detailed information likely to be available in the region. In other countries data availability is poor and where it is available the quality (in terms of coverage, resolution and direct hydrological relevance) is generally low (Kapangaziwiri, 2008). In this study the parameter estimation processes that directly incorporate uncertainty were developed based on the best available data in South African with the expectation that they can be adapted to the other situations obtaining in the region.

4.1.2 Description of the AGIS data

For South Africa, the basin physical property information needed for the estimation of parameters and the uncertainty associated with them was derived from the AGIS land type information (AGIS, 2007). This is currently the best database representing the requisite information for this study and thus formed the basis for the design of these procedures. The AGIS land type maps are originally designed for the assessment of agricultural potential of South African land areas. However, the data can be used as an essential input into the parameter estimation equations. These data are especially useful for the main runoff generation parameters that are expected to be determined from soil and topography characteristics. The procedure (Sililo et al., 2001) for the construction of the land type maps procedure is represented in Figure 4.1.

Terrain units, made up of uniform terrain form, were demarcated using 69 existing 1:250 000 topocadastral maps as background. These were combined with climate and soil maps to delimit the land type areas forming the land type maps at a scale of 1:250 000 (Land Type Survey Staff, 1997). Each land type exhibits a unique combination of soil pattern, macroclimate and terrain form and the boundaries between land types are determined by a change in any one or more of these features. Originally, 52 maps were printed with the land type information on top of the cadastral information but these were later digitized to obtain the electronic coverage of South Africa that exists today (www.agis.agric.za/agisweb/landtypes). AGIS (2007) is an online geo-referenced version of the land type database and provides a full description of any chosen land type for any area in the form shown in Figure 4.2.

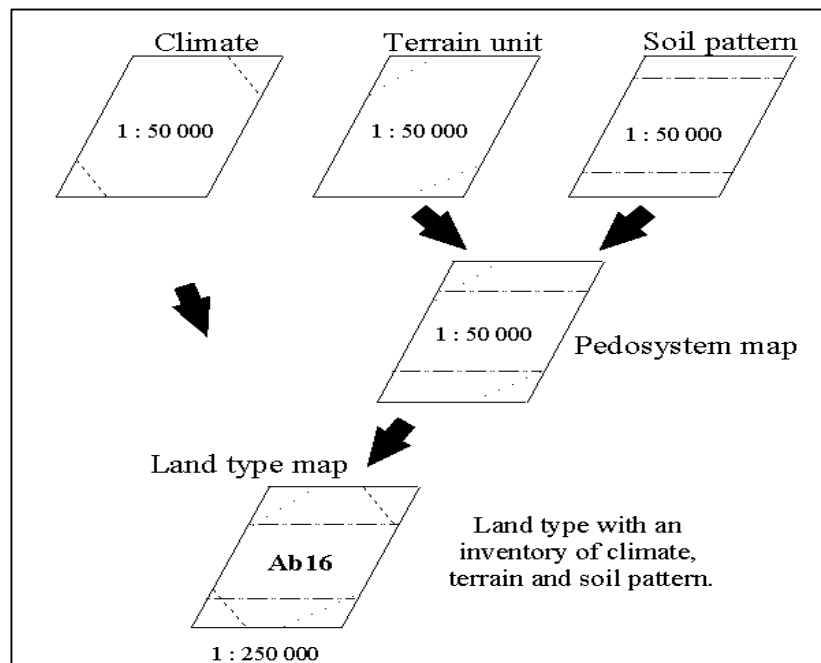


Figure 4.1 The procedure followed for the construction of the land type maps (Sililo et al., 2001)

The AGIS data typically includes the following information:

- ❖ The total area (ha) covered by the land type and the part of this area that is not arable.
- ❖ A brief description is given of the rock type and the geological formations present in the land type in their order of dominance. Information is generally derived from published 1: 250 000 scale geology maps (Geological Survey, 1981) and is used in conjunction with the published 1: 1 million scale geology map of South Africa (Geological Survey, 1984).
- ❖ Up to five terrain units (1 – 5) are used to describe each land type. A profile sketch of the terrain type indicating the land type by its number (Fb132 in Figure 4.2). These terrain units are representations of hilltops/crests, scarps or upper slopes, middle slopes, foot/lower slopes and the valley bottoms. In the parameter estimation procedures only four of these units are considered. For each of these terrain units the following information, relevant to the estimation procedures, is specified:
 - ❖ Area (%) – the percentage of area occupied by each terrain unit within the land type (e.g. 15, 50, 20, and 15% for the terrain units 1, 3, 4 and 5 respectively in Figure 4.2).
 - ❖ Slope (%) – this is given as a range of the percentage slope whose calculations are based on a slope wedge (in Figure 4.2 these are 0-3, 6-12, 2-4 and 0-13 for the terrains 1, 3, 4 and 5 respectively).
 - ❖ Shape of slope – with concave, convex and straight slope forms denoted by X, Y and Z respectively.
 - ❖ Soil information – while the database does not give information on the spatial distribution arrangement of each soil series within a land type, an estimate of the area (%) covered by each soil series within each terrain unit is provided. The soils information provided are the depth range, topsoil and subsoil clay content, texture and type of depth limiting material for each soil series. There is no differentiation of depth within each terrain unit for a specific soil series.
 - ❖ The mechanical limitations associated with each terrain unit are described in terms of the classes given below. The limitations are due to stoniness and/or shallowness.
 - MB0 – no mechanical limitations
 - MB1 – many stones, but ploughable
 - MB2 – large stones and boulders, unploughable
 - MB3 – very shallow soils on rock
 - MB4 – lack of soil

While information on soil hydraulic properties is not explicitly given in the database, it is assumed that these can be inferred from the texture class. The soil texture type information is therefore used to define and quantify some basic soil property values such as infiltration parameters, porosity and permeability based on the literature containing typical values (for example USDA, 1969; Rawls et al., 1982; Schulze et al., 1985).

4.1.3 Description of the GRAII data

The Department of Water Affairs Groundwater Resource Assessment Phase II (GRA II) is based on a simple water balance model for the estimation of groundwater allocation scenarios. It is designed to model a distinct geohydrological or hydro-lithological unit (such as a groundwater flow basin) and to provide a rough, desktop estimate of the status of the groundwater resource and what volume might be abstracted without damaging local surface aquatic ecosystems over the long-term (DWAF, 2005). Algorithms have been developed for the estimation of storage, recharge, baseflow and the impact of present groundwater use has also been recorded. The results include several valuable datasets and maps and provide input to various levels of water resources planning and management. For the purposes of this study the most important data available from the GRAII database relate to the estimates of regional ground water slope, aquifer thickness, transmissivity, storativity and ground water recharge.

GRAII Recharge

Three estimates of groundwater recharge are given in GRAII for each quaternary catchment in South Africa. These values are essentially derivatives of estimates based on the Chloride Mass Balance (CMB) method which assumes that drainage of water is inversely proportional to the chloride content of pore water. This is the most common method used in the country. The method was used in a GIS framework where several GIS layers were used as filters to remove anomalies and introduce local variation to the results of the CMB method. The filters used include saturated aquifer thickness, soil drainage (Schulze, 1997), rainfall seasons, geology, land cover, topography and coefficient of variation of annual precipitation (DWAF, 2005). The resulting recharge values were then calibrated against observations, values reported in the literature or outputs from other more localized methods. The three values in the national database are;

Mean calculated recharge percentage from GRAII - output from GIS calibrated layer: These are the original outputs from the GIS filtered CMB results. They are based on multiple regression techniques applied to CMB output and GIS layers and calibrated against only 42 stations where recharge is calculated by the CMB method. Of the three recharge values given in GRAII, these are the always the largest.

Mean calculated recharge percentage from GRAII - GIS calibrated against Karim Sami's output: These values are derived from the calibration of the CMB output and the GIS filter against the output of Karim Sami. While there is no explanation in the GRAII about the derivation of the Karim Sami values, it is common knowledge that Sami has done extensive work on groundwater recharge estimation (both published and unpublished) in many basins of the country using various methods (for example, Sami and Hughes, 1996; Sami and Murray, 1998; Sami, 1991; 1992 and 1994). The results of these studies were used to calibrate the CMB/GIS filtered outputs. This value is generally the smallest of the three estimates.

Mean calculated recharge percentage from GRAII - GIS calibrated against output from RDM (Resource Directed Measures) office: This value is derived from the calibration of the CMB output and DGIS filters against quaternary based values from the groundwater/surface water interaction (GW/SW) project undertaken for the RDM (Resource Directed Measures) Directorate of the Department of Water affairs (DWA). The final recharge value was adjusted to match the estimated baseflow for the quaternary basins. It is therefore based on assumed base flows, derived using base flow separation procedures and appears to assume that recharge is equivalent to base flow ignoring any evaporation losses.

Experience of use of the values in water resources estimations indicates that hydrological simulations with the two lower values produce more reasonable and consistent results compared to the largest values (Hughes, pers comm.). For the estimation of uncertainty related to the recharge parameter GW, the two lower values were therefore used.

4.2 Estimating the parameter priors

In Bayesian statistical inference a prior probability distribution (often referred to as just the prior) of an uncertain quantity is the probability distribution that

expresses the uncertainty about the quantity before observations are taken into account and used to constrain the prior uncertainty and determine posterior parameter distributions representing behavioural parameter sets. As discussed in Chapter 3 the approach used in this study is to constrain the prior parameter distributions using the measured physical properties (and their uncertainty) coupled with the parameter estimation equations.

The AGIS data are generalized using soil type and terrain units at scales that are smaller than the modelling scale. This generalization is expressed as ranges of slope for each terrain unit and ranges of depth for each soil type. The assumption inherent in the approach used in this study is that these ranges can be used to represent the uncertainty in the appropriate value of any physical property metric to use at the basin scale for the purpose of estimating a model parameter value. Further uncertainty is related to the fact that there are a number of different terrain units and soil types that are associated with a single land type. Where several land types occur within a model spatial unit, additional uncertainty in the estimation of an appropriate parameter value is associated with this added spatial variability (Figure 4.3). The assumption used in this study is that the variations in the physical basin property data represent the uncertainty in the representation of these data at their scale of measurement. These explicit variations at the smaller or sub-basin scale can be used to estimate the uncertainty at the model scale.

The basic tenet of the incorporation of uncertainty into the parameter estimation procedures is to assume some uncertainty in the physical basin attribute data that are used to directly quantify the model parameters. The rationale is that, if the frequency distribution properties of the input physical property data can be established, then it is possible to describe the distribution characteristics of an output parameter. Figure 4.4 is an illustration of this process where the primary data inputs refer to the raw basin characteristic data, measured at smaller scales and most will need to be transformed into their basin scale equivalents (the secondary variables). If the definition of PDFs of the inputs can be successfully defined then it would be possible to sample from these distributions to define distributions for the secondary inputs and, finally, the parameters.

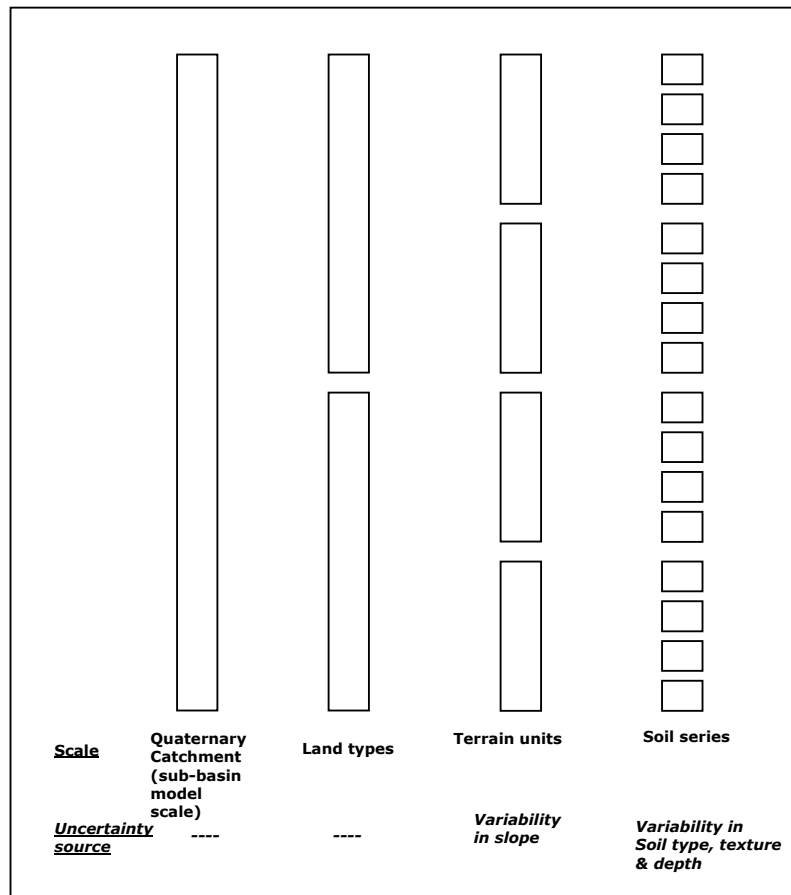


Figure 4.3 An illustration of the complexity of the scale issues arising in the parameter estimation process incorporating uncertainty

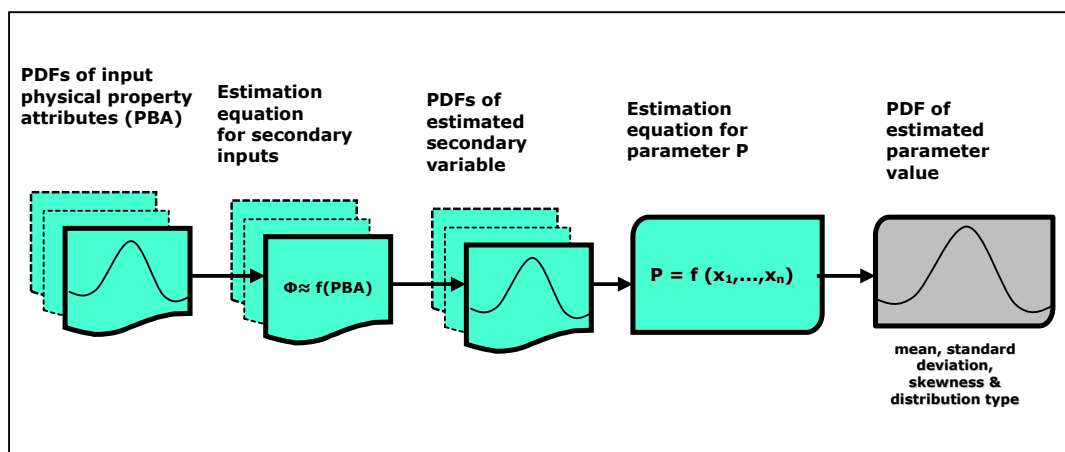


Figure 4.4 The procedure followed for the incorporation of uncertainty in the estimation procedures of the Pitman model parameters

While there exist a number of distribution types for most environmental variables (Munoz-Carpena et al., 2007), it is generally accepted that the means, variances and ranges of the input parameters exert more influence on the output uncertainty than the form of the distribution (Haan et al., 1998). While values of common environmental parameters usually depend on the general variability of the application area selected and the scale (size) for which the measurement is expressed (Hillel, 1998), it is possible to derive marginal PDFs from scientific literature, physical bounds, surveys, expert judgment, and experiments (Saltelli et al., 2005). For instance, “when only the range and a base (effective) value are known, a simple triangular distribution can be used, while in the case when values seemed distributed equally along the parametric range, a uniform distribution is recommended” (Munoz-Carpena et al., 2007). In this study, the physical properties were assumed to have reasonably centrally distributed frequencies and the normal probability distribution was assumed to adequately describe the frequency characteristics of the raw physical basin data in most cases. However, it is noted that this assumption is difficult to confirm without additional detailed field observations. The exception is where a large range of slopes occur within a terrain unit with very steep maximum values. In this case a log-normal distribution was assumed. The posterior distributions of the secondary variables or the resultant parameters are then determined by the combined effect of the input distributions. To obtain the distributions of the secondary variables and the resultant parameters, Monte Carlo sampling was used. Monte Carlo sampling is a common random search method that explores a given space (e.g. an ensemble of inputs or an *a priori* distribution) and is regarded as one of the most efficient sampling methods as it can cover the whole search domain. In simple terms Monte-Carlo sampling refers to generating repetitive solutions of an equation (or model) with randomly sampled input variables from defined probability distributions (e.g. uniform or normal, with or without transformation of the data). The outputs can be analysed to determine the statistical properties of the estimation variable. In this study three statistical measures are calculated from the samples of the secondary variables or parameters; the mean, standard deviation and skewness. There are cases where the estimation equations are non-linear and despite normally distributed inputs, the output distributions can be skewed. Experience has indicated that with environmental variables the skewness is almost always positive or the distribution is near normal. Therefore, whenever the calculated skewness was greater than 2.5 a log-normal PDF was assumed. The choice of the value 2.5 used for the definition of log-normal distribution is somewhat arbitrary but appears to be appropriate. The standard deviations of the

resultant secondary variables or parameter values then represent the extent of uncertainty in their estimates. In some instances the secondary variables are components of some parameters e.g. ST_{soil} and ST_{unsat} which are the two parts that make up subsurface moisture store capacity parameter ST (Kapangaziwiri and Hughes, 2008).

In general the estimation of a normally distributed uncertain parameter, P , can be summarized as in Figure 4.4. This can be written mathematically as:

$$N[\mu_P, \sigma_P] \approx f \{N[v_i(\mu_i, \sigma_i)]\}, \text{ for } i = 1, 2, \dots, n$$

where a posterior normal distribution of the parameter P , with mean μ_P , and standard deviation σ_P is conditioned on the prior distributions of the uncertain input variables v_i with mean μ_i and standard deviation σ_i and n is the number of input variables required to estimate P .

In order to simplify the estimation of the secondary variables and/or parameters and to better manage the input data and calculations, a Delphi program has been developed. Default values for some of the variables (for example transmissivity, porosity and storativity) are provided based on descriptive characteristics based on, for example, the degree of fracturing in hard rocks, or the relative permeability in primary aquifers. These default values are based on experience and information obtained from various literature sources but can also be overwritten if more reliable and site specific information about a variable is available. Figure 4.5 is an illustration of the input data requirements for the parameter estimation process that incorporates uncertainty.

The diagram shows some of the primary input data that are required as well as some of the secondary basin data that are calculated. While the majority of the basin characteristic data are obtainable from the AGIS database, additional primary data required for the parameter estimation process should be obtained from any other suitable source. The full list of all the primary data is given below. Most of the estimation equations and their input requirements are fully discussed (and conceptually justified) in Kapangaziwiri (2008) and have been adapted from those used by Hughes and Sami (1994) in the development of parameter estimation approaches for the daily time step VTI model. Some of the input variables do not have uncertainty associated with them. This is not because they can be estimated without uncertainty, but to simplify some of the estimation

processes and because they are used with other variables that do have uncertainty definitions.

Four terrain units: The AGIS land type data contains a maximum of five terrain units for each land type. The primary data inputs only consider four slope units which are given as the top, middle and bottom slopes, and the valley floor. The percentage of the total sub-basin area covered by each of these terrain units is a primary input. If there is more than one land-type in a sub-basin the primary input is therefore an area weighted average of the distribution of the different terrain units.

Parameter Estimation for the Pitman model (GWV3)

PRIMARY Basin data
Columns represent either:
Soil information for four terrain units or
Mean and standard deviation for sub-basin as a whole.
Right click on soil texture rows to select the appropriate texture.

Property	Top	Mid	Bottom	Valley
% Area	35	50	10	5
Min. Slope (%)	0	6	3	0
Max. Slope (%)	3	10	6	2
S1 % of Unit	45	46	35	0
S1 Min. Depth	400	0	0	0
S1 Max. Depth	600	0	0	0
S1 Texture	SCILm		2	
S2 % of Unit	25	30	20	10
S2 Min. Depth	500	0	0	0
S2 Max. Depth	800	0	0	0
S2 Texture	LmS		1	
S3 % of Unit	10	15	10	0
S3 Min. Depth	200	0	0	0
S3 Max. Depth	500	0	0	0
S3 Texture	LmS		1	
S4 % of Unit	10	5	0	0
S4 Min. Depth	300	0	0	0
S4 Max. Depth	600	0	0	0
S4 Texture	LmS		1	
S5 % of Unit	5	4	15	0

SECONDARY Basin data
Columns represent means and standard deviations of the estimates.
Double click on any row or column to calculate the estimates from the primary data.

Property	Mean Value	SDev Value	Skewness	Dist. Type
Basin Slope (%)	5.045	0.479	0.046	1
Upper Slope (% Area)	35.000			
Mid Slope (% Area)	50.000			
Valley Bottom (% Area)	15.000			
Upper slope S. Depth (mm)	540	27.315	0.025	1
Mid Slope S. Depth (mm)	536	29.375	-0.084	1
Valley Bottom S. Depth (mm)	600	28.675	0.001	1
Soil Porosity	0.364	0.061	0.014	1
Vert. Variation (%)	82			
Soil K	0.593	0.062	0.160	1
Soil K var	0.015			
Soil C	179.142	31.358	0.141	1
Soil C var	105.526			
Soil Perm. (mm/h)	27.603	11.188	0.154	1
ST Soil (mm)	164.181	27.907	0.067	1
FT soil (mm/month)	1.666	0.703	0.404	1
Regional GW slope (%)	1.0			
Drainage Vector slope (%)	6.4			
Storativity (*1000)	5.0	0.5		
Depth to GW(m)	25.0			

Mean Storm Duration (h)	6.0			
Mean Annual Evap. (mm)	1400.0			
Mean Ann. Recharge (mm)	9.6	15		
% Area of Dominant Veg.	80.0			
Dominant Vegetation	Summer		Winter	
Proportions of Dom. Veg.	Low Est.	High Est.	Low Est.	High Est.
Dense Forest	0.0	0.0	0.0	0.0
Bush/Sparse Forest	0.1	0.3	0.1	0.3
Dense Crop/Ground Cover	0.6	0.5	0.6	0.5
Sparse Crop/Ground Cover	0.3	0.2	0.3	0.2
Bare Soil	0.0	0.0	0.0	0.0
% Area of Secondary Veg.	20.0			
Secondary Vegetation	Summer		Winter	
Proportions of Sec. Veg.	Low Est.	High Est.	Low Est.	High Est.
Dense Forest	0.6	0.7	0.6	0.7
Bush/Sparse Forest	0.4	0.3	0.4	0.3
Dense Crop/Ground Cover	0.0	0.0	0.0	0.0
Sparse Crop/Ground Cover	0.0	0.0	0.0	0.0
Bare Soil	0.0	0.0	0.0	0.0

Soil K	0.593	0.062	0.160	1
Soil K var	0.015			
Soil C	179.142	31.358	0.141	1
Soil C var	105.526			
Soil Perm. (mm/h)	27.603	11.188	0.154	1
ST Soil (mm)	164.181	27.907	0.067	1
FT soil (mm/month)	1.666	0.703	0.404	1
Regional GW slope (%)	1.0			
Drainage Vector slope (%)	4.2			
Storativity (*1000)	2.0	0.2		
Depth to GW(m)	25.0			
Fract. Zone Trans. (m2/d)	1.0	0.2		
ST Unsat (mm)	9.942	4.704	-0.189	1
FT Unsat (mm/month)	3.188	1.578	-0.945	1
Moisture content SD (%)	60.410	5.260	-1.942	1
Dominant LAI (Summer)	1.543	0.094	-0.261	1
Dominant LAI (Winter)	1.544	0.094	-0.278	1
Secondary LAI (Summer)	4.300	0.045	0.001	1
Secondary LAI (Winter)	4.300	0.045	0.013	1

Calculate Parameters Output Results Finished

0% Reload From File No File

Figure 4.5 Screenshot of the input primary data for the estimation of parameter with uncertainty

The minimum and maximum slope, given as a percentage, for each of the terrain units considered. The range of the slope values is taken as a measure of the uncertainty. The slope estimates are assumed to be normally distributed and that the minimum and the maximum values given in AGIS represent the 5th and 95th percentiles of the cumulative distribution.

Soil types: Five different soil types can be specified, each with an associated depth range and texture class. No differentiation of soil depth across the different terrain units is given in the AGIS data. Differences in soils across different terrain units are specified as the proportion of the soil type lying in each terrain unit. For each soil, the texture class has to be specified. This study makes use of 5 broad soil texture classes which are sands, loamy sands, sandy clay loams, sandy clays and clays. The frequency characteristics of the soil depths are assumed to be normally distributed with the minimum and maximum values representing the 5th and 95th percentiles of the cumulative PDF.

A vertical variability factor (%) for the soil is included. This is a percentage value that is intended to represent the assumed reduction in permeability and porosity with depth. For instance the vertical variability factor for a duplex soil would be expected to be low. There is no uncertainty assumed for this input.

Indices of the surface cover and cover variability specified for the top, middle and bottom slopes. The surface cover varies from well-vegetated (index 0), through moderately vegetated (1) to crusting (2), while its variability is from low (0), through moderate (1) to high (2). These factors are important for the estimation of the infiltration parameters and can be obtained from an understanding of the vegetation cover. Also required is a representation of the *organic content* of the soil, its *structural* development and the extent of *macro pore* development specified for each sub-basin. These factors are input without uncertainty. The variation of these soil factors is given as an index value from low (0) to high (2) and are used in the estimation equation of the soil permeability (a secondary variable).

An estimate (without uncertainty) of the *regional groundwater slope (%)* obtained from the GRAII (DWAF, 2005) database.

The *vertical and lateral drainage* components of subsurface water movement (no uncertainty). This concept is based on the understanding that water in the

fractures within the unsaturated zone between the soil and the water table is prone to two directional components - a vertical one contributing directly to recharge of the saturated ground water zone and a lateral one that could contribute to the re-emergence of subsurface water at a spring or seep (Hughes, 2010). The percentage values of these vertical and horizontal components need to be specified based on the geological characteristics of the unsaturated zone. These characteristics include the type of geological material, the extent of fracturing or weathering of the rock formation or its permeability. If the formation is completely weathered, then it is not feasible to have a lateral flow component unless the gradient is very steep. Deep weathered rock material does not support springs above the level of ground water. While default values based on limited knowledge are available, these are very generalized and can be over-written if more reliable data are available. It is acknowledged that appropriate values will be difficult to estimate in many basins.

The *storativity* of the aquifer which will depend on the characteristics of the underlying rock formation. The representation of uncertainty is done through the specification of the standard deviation of the input value in an assumed Normal distribution. The standard deviation of storativity is by default, set at 10% of the mean value which can be changed should better information be available.

An estimate of the *depth to ground water (m)* whose approximate value can be found in the GRAII database given as aquifer thickness. While these are not exactly the same thing, the GRAII aquifer thickness values are the only source of information and have been used in previous modelling studies with success. The value of depth to groundwater is given without estimation of uncertainty.

The *transmissivity (m^2/d)* of the unsaturated fracture zone estimated with a standard deviation set at a default value of 20% of the input value.

Basin *drainage density (km/km^2)* with default standard deviation set at 10% of the input value. This input is a measure of channel length and can be estimated from topographic maps. In this study its estimation included all potential drainage lines (identified by contour convergence) that are assumed to receive flow under conditions of basin saturation. While this makes the drainage densities higher than the use of 'blue' lines, it was assumed to be an appropriate approach given the use of the variable in the estimation of the maximum interflow rate (parameter FT) when soil moisture storage is full (Kapangaziwiri, 2008).

The *mean monthly rainfall (mm)* for the basin and the *maximum rainfall (mm)* estimated from the time series of the available records. Related to this is the mean monthly *number of rain days* and the *mean duration (in hours)* of rainfall events in the area. The International Water Management Institute (IWMI) Online Climate Service Model (<http://wcatlas.iwmi.org/Default.asp>) can provide reasonable estimates of number of rain days for any chosen point on the globe. In areas where, national records are available, these can be used instead. Also required is the mean *annual potential evaporation (mm)* for the basin. These climatic variables are used in the estimation of the surface runoff parameters of the model.

The minimum and maximum mean *annual recharge (mm)* values. The values used are taken from the GRAII database (DWAF, 2005). From the three values that are available per basin, the two lower ones are used since experience has shown that the largest is most unreliable. The two values are taken to represent the 10th and 90th percentiles of a Normal distribution of the mean annual recharge.

It is also required to include the characteristics of the two dominant vegetation types in the basin (input to represent dominant and secondary vegetation). The area covered by each vegetation type is given as a percentage of the total basin area. A description of the types of vegetation cover is expressed in terms of five predefined vegetation classes. These classes are Dense Forest, Bush, Dense Crop/Groundcover, Sparse Groundcover and Bare Soil. To account for uncertainties in the estimation of the interception parameters, high and low estimates of the vegetation types are given for both winter and the summer seasons (Figure 4.6). Note that summer and winter values are equal since seasonal differences were found to be insignificant.

% Area of Dominant Veg.	80.0			
Dominant Vegetation	Summer		Winter	
Proportions of Dom. Veg.	Low Est.	High Est.	Low Est.	High Est.
Dense Forest	0.0	0.0	0.0	0.0
Bush/Sparse Forest	0.1	0.3	0.1	0.3
Dense Crop/Ground Cover	0.6	0.5	0.6	0.5
Sparse Crop/Ground Cover	0.3	0.2	0.3	0.2
Bare Soil	0.0	0.0	0.0	0.0
% Area of Secondary Veg.	20.0			
Secondary Vegetation	Summer		Winter	
Proportions of Sec. Veg.	Low Est.	High Est.	Low Est.	High Est.
Dense Forest	0.6	0.7	0.6	0.7
Bush/Sparse Forest	0.4	0.3	0.4	0.3
Dense Crop/Ground Cover	0.0	0.0	0.0	0.0
Sparse Crop/Ground Cover	0.0	0.0	0.0	0.0
Bare Soil	0.0	0.0	0.0	0.0

Figure 4.6 An illustration of the vegetation input data that is used to estimate the variability of the interception parameters.

It should be noted that in some instances there are default mean values for input data and their estimates of uncertainty, these are representations of expected values drawn from previous studies, literature or experience. These defaults can be overwritten where more recent and reliable information is available. Similarly, default values for the standard deviation of some variables are included (storativity, transmissivity, for example). If a user feels confident about their ability to estimate these values, the default standard deviation values can be modified. The following sections explain the estimation of the secondary variables and the uncertain parameters from the given primary data. The approach taken is to explain the derivation of the secondary variables at the same time as the parameters they relate to. The estimation equation for the parameter is given first, followed by a description of how uncertainty is incorporated into the equation. The explanation is preceded by a brief synopsis of the estimation process as explained in the previous work (Kapangaziwiri, 2008). In all of these sections, the following expressions and terminology will be used:

- ❖ Monte-Carlo methods are used to sample from the primary or secondary variable distributions. During sampling, if a sample is generated that is not feasible (for example, negative values) it is rejected and the sampling is repeated. It is quite possible, for example, for the sampling process to generate negative values if the variable range is input as 0 – 100 mm and these are taken to represent 98% of a Normal distribution. However, negative values cannot be used in the estimation equation.

- ❖ For the secondary variables and parameters that are determined from the estimation equation outputs, the mean, standard deviation and skewness are calculated from the sample values. If the skewness exceeds 2.5, the process is repeated using natural logarithm transformed values and the output values are the back-transformed means and standard deviations and the original skewness value of the untransformed distribution.
- ❖ The mean and standard deviation of the Normal or log-Normal PDFs will be represented by μ and σ respectively.
- ❖ The full description of a PDF will be given by $N[\mu, \sigma]$, where N indicates a Normal probability distribution.
- ❖ The description of a single sample taken from a normal distribution is given as $N[\mu, \sigma]_k$.
- ❖ For any specific variable (VAR), its mean and standard deviation will be given, respectively, as μ_{VAR} and σ_{VAR} . For instance, μ_{DEP} and σ_{DEP} represent the mean and standard deviation of soil depth (DEP).

4.2.1 Estimating uncertainty for the parameter ST

ST is conceptually viewed as a sum of two subsurface storages – the storage of the soil (ST_{soil}) and that of the zone of intermittent saturation that lies between the soil and the water table (ST_{unsat} , Kapangaziwiri, 2008).

$$ST = ST_{soil} + ST_{unsat} \dots\dots\dots 4.1$$

4.2.1.1 Estimating uncertain ST_{soil}

The soil moisture storage capacity at saturation (ST_{soil}) was deemed to be influenced by the porosity (POR %) and depth (DEP mm) of the soil. A correction factor, subjectively determined for each terrain unit, to account for the variation of porosity with depth (VVAR %) was also included (Kapangaziwiri, 2008). The final equation for the estimation of this moisture component was given by:

$$ST_{soil} \text{ (mm)} = DEP * POR * VVAR/100 \dots\dots\dots 4.2$$

POR is a basin area-weighted value dependent on the distribution of the soil texture classes and DEP is a mean estimate based on the percentage areas of the basin occupied by three main topographic units (upper slope, mid slope and valley bottom). DEP was estimated using the following algorithm:

$$DEP = \sum_{i=1}^3 (DEP_i * TAREA_i) \dots\dots\dots 4.3$$

where TAREA_i is the area of the terrain unit i. The derivation of the uncertain ST_{soil} (STS) is therefore estimated as:

$$N[\mu_{STS}, \sigma_{STS}] = N[\mu_{DEP}, \sigma_{DEP}] * N[\mu_{POR}, \sigma_{POR}] * VVAR/100 \dots\dots 4.4$$

where μ and σ are the means and standard deviations of the distributions of the variables POR and DEP (shown by subscripts). VVAR is not considered with uncertainty as its uncertainty effect is assumed to be negligible in most cases, compared to the other variables in Equation 4.4. In the case that uncertainty is necessary, a uniform distribution (specifying maximum and minimum possible values) can easily be used. The following sections explain the determination of the uncertain soil depth and porosity estimates.

Estimating the distribution of soil depths

The estimation of uncertainty is based on the range of the depth values for each of the 5 soil types. A distribution of soil depths is determined for each of the terrain units. Soil depth was assumed to be normally distributed with mean μ_{DEP} and standard deviation σ_{DEP} . The first step is to determine the PDFs of soil depth for each of the terrain units. For each soil type, j, the mean of the soil depth, μ_{DEP_j} , is given simply as:

$$\mu_{DEP_j} = (DEP_j \text{ (min)} + DEP_j \text{ (max)}) / 2 \dots\dots\dots 4.5$$

where min and max are the minimum and maximum soil depth as input from the AGIS database. For instance, the mean soil depths for the five soil types (1-5) given in Figure 4.4 are 500, 650, 350, 450 and 900 (Table 4.1).

It was assumed that the range of depths for each soil type represents the 98% limits of the normal distribution of all possible depths, equivalent to 2.33 standard deviations about the mean value. The standard deviation of each soil type j, σ_{DEP_j} can thus be calculated as:

$$\sigma_{DEP_j} = [(\mu_{DEP_j} - DEP_j \text{ (min)}) + (DEP_j \text{ (max)} - \mu_{DEP_j})] / (2 * 2.33) \dots\dots\dots 4.6$$

This results in standard deviation values for the soil types 1 to 5 of 42.9, 64.4, 64.4, 64.4 and 42.9 respectively (Table 4.1).

Table 4.1 The distributions of soil depths and the proportions of soil type in terrain unit (A_{ij}) used for the area weighting in the soil depth calculations

Soil type	Depth range	Mean value	Standard deviation	Top A_{1i}	Middle A_{2i}	Valley /Bottom A_{3i}
1	400 - 600	500	42.9	0.47	0.46	0.39
2	500 - 800	650	64.4	0.26	0.30	0.33
3	200 - 500	350	64.4	0.11	0.15	0.11
4	300 - 600	450	64.4	0.11	0.05	0.00
5	800 - 1000	900	42.9	0.05	0.04	0.17

To establish the mean μ_{DEP_i} and σ_{DEP_i} for each of the terrain units, the proportions of areas of soil type j occurring in each terrain unit i (A_{ij}) are calculated. The net result is a matrix of area proportions given in Table 4.1. These proportions are then used as weights in the calculation of μ_i and σ_i . A Monte Carlo procedure was used to generate 2000 samples from the Normal probability distributions of depths within the soil types and the samples weighted by the relevant proportion A_{ij} :

$$DEP_{ik} = \sum_{j=1}^5 N[\mu_{DEP_j}, \sigma_{DEP_j}]_k * A_{ij} \dots\dots\dots 4.7$$

where DEP_{ik} represents the k th sample of soil depth from terrain unit i . From the 2000 combined samples the mean, standard deviation, skewness and distribution type of the soil depths are determined for each of the three terrain units i.e. $N[\mu_{DEP_i}, \sigma_{DEP_i}]$. These are the distributions of three secondary variables that represent the spatial distribution of soil depths in the basin.

Estimating the distribution of porosity (POR)

The variable POR is a soil hydraulic property and was determined from the 5 texture classes for the whole sub-basin. An area weighting procedure is used based on the proportion of area occupied by each soil type across all terrain units to take into account the distributions and influences of the different soil units. For the five texture classes used (sandy (Sa), loamy sands (LmSa), sandy clay loams

(SaCILm), sandy clay (SaCl) and clays (Cl)), the assumed mean values of porosity used in this study are 40%, 42%, 33%, 32% and 39% respectively (Kapangaziwiri, 2008). The standard deviation was fixed at an arbitrary value of 5% of the mean for each soil type.

5000 Monte Carlo samples were taken from the porosity distributions within the soils across all the terrain types. The number of samples taken from each terrain type depends on the proportion of the terrain that is occupied by the soil type. If 30% of terrain is covered by a particular soil type then 30% of the samples are taken from that terrain. The distribution properties of the basin porosity are determined from the 5000 samples. This distribution is written as $N[\mu_{POR_i}, \sigma_{POR_i}]$.

Estimating the vertical variation (VVAR)

The variation of the soil porosity with depth (VVAR) is a weighted average for the basin that is used with no uncertainty. This is taken as a mean value across the terrain units based on the proportion of the basin occupied by each of the terrain units. For the example, from the data in Figure 4.5, it is calculated as follows:

$$VVAR = (0.35 \times 90) + (0.5 \times 80) + (0.15 \times 70) + (0.05 \times 70) = 82\% \dots\dots\dots 4.8$$

Final estimation of ST_{soil} PDF

The final distribution of ST_{soil} is then determined through a combination of samples of the terrain unit soil depths and the basin porosity. 1500 area weighted Monte Carlo samples are taken from each of the distributions of the terrain units and combined to an equally sized sample of basin porosity together with the VVAR factor to generate samples of ST_{soil} according to the relationship:

$$(ST_{soil})_k = \sum_{i=1}^3 \{N[\mu_{DEP_i}, \sigma_{DEP_i}]_k * TAREA_i\} * N[\mu_{POR_i}, \sigma_{POR_i}]_k * VVAR/100 \dots 4.9$$

where k is the kth sample and the mean, standard deviation, skewness and posterior distribution type of ST_{soil} are determined from the 1500 samples.

4.2.1.2 Estimating uncertain ST_{unsat}

The estimation of ST_{unsat} is based on depth to the water table (DGW m), the storativity (St) of the unsaturated zone and a factor (Ratio) that accounts for the

orientation of the fracture drainage vector slope (VS) relative to the regional ground water slope (GS) and the basin surface slope (BS). The concept of VS stems from the understanding that percolating water through the unsaturated zone is subject to both vertical and lateral flow components whose vector sum is VS. The Ratio is given by:

$$\text{Ratio} = [\text{Tan}(\text{BS}) - \text{Tan}(\text{VS})] / [\text{Tan}(\text{BS}) - \text{Tan}(\text{GS})] \dots\dots\dots 4.10$$

and the equation for the estimation of ST_{unsat} is:

$$\text{ST}_{\text{unsat}} = \text{DGW} * 1000 * \text{St} * \text{Ratio} \dots\dots\dots 4.11$$

In this study DGW is estimated without uncertainty. Mean basin values of storativity are obtained from the GRAII database (DWAF, 2005). These mean values are assumed to be normally distributed with a standard deviation fixed at a default value of 5% of the mean. The only other variable that is estimated with uncertainty is BS. This is estimated from the slope information from the AGIS (2007) database.

Estimating the PDF of basin slope (BS)

The calculation is based on 4 of the 5 terrain units from the AGIS land type data. If there are five terrain units in any given basin, then any two can be combined depending on the closeness of the information for the two slopes. In most cases the bottom slopes and the valley floors have been combined. The mean basin slope for each terrain unit (μSLOPE_i) is calculated from the maximum and minimum as follows:

$$\mu\text{SLOPE}_i = (\text{max}_i + \text{min}_i) / 2 \dots\dots\dots 4.12$$

with max_i and min_i being the maximum and minimum slope values for terrain unit i . A minimum slope value of 0.1% is assumed for all slopes reported as zero. The standard deviation of the slopes for each of the terrain units i is based on the assumption that the maximum and minimum slopes represent 98% of a Normal distribution. These limits represent 2.33 standard deviations about the mean of a fairly large sample size and the standard deviation is thus determined as:

$$\sigma\text{SLOPE}_i = [(\text{max}_i - \mu\text{SLOPE}_i) + (\mu\text{SLOPE}_i - \text{min}_i)] / (2*2.33) \dots\dots\dots 4.13$$

The result is a Normal distribution, defined by mean μ_{SLOPE_i} and standard deviation σ_{SLOPE_i} , of slopes for each of the four terrain units. Where the maximum slope is greater than 40%, natural logarithm transformations of the slope values are used and the distribution type for that terrain unit is assumed to be log-Normal. From these distributions of secondary variables, 5000 Monte Carlo area weighted samples are generated to estimate the distribution of the slope of the basin. The weighting is based on the proportion of the basin covered by each terrain unit. Using the example data in Figure 4.5, 1750, 2500, 500 and 250 will be taken from terrain units 1, 2, 3 and 4 which cover 35%, 50%, 10% and 5% of the basin respectively. The mean, standard deviation, skewness and distribution type of BS are then determined from these 5000 samples.

Estimating PDF of ST_{unsat}

5000 samples of the ratio are then generated through Monte Carlo samples from the distribution of the basin slope using:

$$[Ratio]_k = [Tan(N[\mu_{BS}, \sigma_{BS}]_k) - Tan(VS)] / [Tan(N[\mu_{BS}, \sigma_{BS}]_k) - Tan(GS)] \dots\dots\dots 4.14$$

where k is the k^{th} of 5000 samples. These samples were then combined with an equal number of samples from the distribution of storativity to generate 5000 samples of ST_{unsat} . From these the mean, standard deviation, skewness and distribution type were determined.

4.2.1.3 The final PDF of parameter ST

Finally 5000 samples are taken from the distributions of both ST_{soil} and ST_{unsat} to generate 5000 samples of the parameter ST. The final PDF of ST can thus be written as:

$$N[\mu_{ST}, \sigma_{ST}] = N[\mu_{STS}, \sigma_{STS}] + N[\mu_{STU}, \sigma_{STU}] \dots\dots\dots 4.15$$

where the subscripts STS and STU refer the components ST_{soil} and ST_{unsat} respectively. The mean, standard deviation, skewness and distribution type for the parameter ST are determined from these 5000 samples.

4.2.2 Estimating the uncertainty associated with the parameter FT

The parameter FT (mm month⁻¹) refers to the depth of interflow when the basin is saturated. The approach adopted for its quantification from physical basin properties uses the same two components (soil and unsaturated) that are used for ST:

$$FT = FT_{\text{soil}} + FT_{\text{unsat}} \dots\dots\dots 4.16$$

4.2.2.1 Estimating uncertain FT_{soil}

FT_{soil} (mm month⁻¹) was estimated using a combination of basin average values of slope (BS %), soil permeability (K m d⁻¹), soil depth in the lower topographic units (DEP mm) and an assumed contributing channel length (based on drainage density, DD km km⁻²). The estimation equation for FT_{soil} is given by:

$$FT_{\text{soil}} = CA * K * 30 * BS / 100000 \dots\dots\dots 4.17$$

where CA is the contributing area per unit basin area estimated as;

$$CA \text{ (m}^2 \text{ km}^{-2}\text{)} = 2 * DD * DEP \dots\dots\dots 4.18$$

Incorporating uncertainty into the estimation of this component of interflow requires that the uncertainties associated with the estimation of BS, DEP, K and drainage density be accounted for. The derivation of the uncertain FT_{soil} can be presented as:

$$N[\mu_{\text{FTS}}, \sigma_{\text{FTS}}] = 60 * N[\mu_{\text{DD}}, \sigma_{\text{DD}}] * N[\mu_{\text{DEP}}, \sigma_{\text{DEP}}] * N[\mu_{\text{K}}, \sigma_{\text{K}}] \\ * N[\mu_{\text{BS}}, \sigma_{\text{BS}}]/100000 \dots\dots\dots 4.19$$

with μ and σ being the means and standard deviations of the distributions of the variables DD, DEP, K and BS and FTS refers to FT_{soil}. The derivation of the distribution functions of soil depth and basin slope within a basin were explained in Sections 4.2.1.1 and 4.2.1.2. Only the distributions of DD and K will be explained in detail here.

Estimating the PDF of drainage density (DD)

Drainage density (DD) is a measure of channel length and its mean value can be estimated from topographic maps or any available literature. In the parameter estimation procedures the derivation of mean drainage density (μ_{DD}) included all potential drainage lines (identified by contour convergence on a topographic map) that are assumed to receive flow under conditions of basin saturation. This is deemed a realistic assumption under basin saturation conditions when seasonal streams emerge and result in drainage densities that are higher than mere use of 'blue' lines (Kapangaziwiri, 2008). Uncertainty in drainage density estimates was assumed to be normally distributed ($N[\mu_{DD}, \sigma_{DD}]$) with a default standard deviation (σ_{DD}) fixed at an arbitrary value of 10% of the mean.

Estimating the PDF of Permeability (K)

For each of the input soil types j , the mean permeability in each terrain unit i (μ_{K_i}) is calculated using the following equation taken from Hughes and Sami (1994):

$$(\mu_{K_i}) = \sum_{j=1}^5 e^{(PI_j * 0.55 - 0.054)} \dots\dots\dots 4.20$$

where PI_j is some assumed index of permeability (PI) of soil type j estimated from the soil's characteristics and is given by:

$$PI_j = M + 0.5 * (F+G+H) + Y \dots\dots\dots 4.21$$

where

$$M = 0.09A + 0.05B + 0.02C + 0.015D + 0.01E \dots\dots\dots 4.22$$

and A to E are percentage areas of the basin covered by sandy (A), loamy sand (B), sandy clay loam (C), sandy clay (D) and clay (E) soils, while F, G and H are assumed to vary from low (0) to high (2) and represent the level of macro-pore development (F), the organic content (G) and the structural development of the soil (H). Y represents the sand grade of the soil, which has been fixed at an index value of 1 in this study. Thus, for a given soil or soil combination within a terrain unit i , a mean permeability (μ_{K_i}), a secondary variable, is calculated. The mean basin permeability (μ_K) is then calculated as an area weighted value based on the proportion of the area of each terrain unit occupied by a soil of type j . The standard deviation for normally distributed permeability per terrain unit i (σ_{K_i}) is fixed at a default value of 10% about the mean value. From 5000 Monte Carlo

generated area weighted samples the distribution ($N[\mu K, \sigma K]$) of basin permeability (K) is determined.

4.2.2.2 Final PDF of FT_{soil}

For the final PDF of FT_{soil} , the 5000 area weighted samples of soil depth from each terrain unit are first combined with those of basin slope. It was noted that due to the independence assumed for the sampling process it is possible to get conceptually implausible combinations of soil depth and basin slope. For example, uncontrolled sampling can produce combinations of steep slopes with deep soils, which are unlikely and should be excluded from the sampling process to avoid inappropriate skewness in the PDF of FT_{soil} . This was achieved with an equation that generates a maximum possible soil depth for any given slope over 20%:

$$DEP_{max} = 85000 / BS^{1.7} \dots\dots\dots 4.23$$

Using this equation results in maximum soil depths for slopes of 20, 30, 40 and 60% being limited to 520, 260, 160 and 80mm respectively. In the absence of sufficient real data on the relationships between maximum soil depths and topographic slope, equation 4.13 has been based on the author's intuition and certainly achieves the objective of preventing excessively high FT_{soil} values in the sample. Where an unacceptable sample is obtained, it is rejected and another sample is taken to replace it. The 5000 samples generated from the combination of depth and slope are then combined with equally sized samples from the distributions of drainage density and permeability, resulting in 5000 samples of FT_{soil} (FTS) from which the basin mean, standard deviation, skewness and distribution type are calculated. This defines the PDF of FTsoil as $N[\mu FTS, \sigma FTS]$.

4.2.2.3 Estimating uncertain FT_{unsat}

The estimation of FT_{unsat} ($mm\ month^{-1}$) is based on the use of basin averages for the vector slope of the fracture zone (VS %) and transmissivity ($T\ m^2\ d^{-1}$) of the subsurface rock formations:

$$FT_{unsat} = 2 * DD * T * 30 * VS / 100 \dots\dots\dots 4.24$$

Of the input basin physical variables, VS is estimated without uncertainty and the uncertain, normally distributed FT_{unsat} (FTU) is expressed as:

$$N[\mu_{FTU}, \sigma_{FTU}] = 2 * N[\mu_{DD}, \sigma_{DD}] * N[\mu_T, \sigma_T] * 30 * VS/100 \dots\dots 4.25$$

where the distribution $N[\mu_{DD}, \sigma_{DD}]$ was already referred to in Section 4.2.2.1. μ and σ are both given in mm month⁻¹.

Estimating the PDF of transmissivity (T)

The transmissivity variable accounts for the variability of the underlying geology and its basin mean (μ_T) value reflects the hydraulic characteristics of subsurface formations. Table 4.2 lists the default values for μ_T and σ_T based on typical geological conditions in the region. The standard deviation values have been fixed at 20% of the mean in the absence of any real data. In cases where more accurate data are available, these can be over-written. The distribution of T can thus be written as $N[\mu_T, \sigma_T]$.

Table 4.2 Default values of transmissivity for different unsaturated zone characteristics

Material	Mean	Standard Deviation
Fractured material – high fracture density	5.0	1.0
Fractured material – moderate fracture density	2.5	0.5
Fractured material – low fracture density	1.0	0.2
Permeable material – high permeability	2.0	0.4
Permeable material – moderate permeability	1.0	0.2
Permeable material – low permeability	0.5	0.1

4.2.2.4 The PDF of FT_{unsat}

The final distribution of FT_{unsat} is determined from 5000 Monte Carlo samples. These are generated from the combination of samples of drainage density and transmissivity with a fixed value of VS. From these 5000 samples the basin mean, standard deviation, skewness and distribution type of FT_{unsat} are calculated.

4.2.2.5 The final distribution of parameter FT

The posterior distribution function of the parameter FT is derived from a combination of 5000 Monte Carlo samples each taken from the distributions of FT_{soil} and FT_{unsat} using the following relationship:

$$N[\mu_{FT}, \sigma_{FT}] = N[\mu_{FTS}, \sigma_{FTS}] + N[\mu_{FTU}, \sigma_{FTU}] \dots\dots\dots 4.26$$

This results in 5000 samples for the population of values for model parameter FT, from which the basin mean value, standard deviation, skewness and distribution type are determined.

4.2.3 Estimating uncertainty in parameter POW

POW represents the non-linearity in the relationship between runoff (Q mm month⁻¹, with a maximum value of FT) and moisture storage (S mm with a maximum value of ST) and is assumed to be influenced by the moisture re-distribution capacity within a sub-basin as it dries out. A procedure similar to that used by Hughes and Sami (1994) has been adopted and it is based on the probability distributed principle (Moore, 1985) that suggests that the overall sub-basin moisture content (S) can be represented by a frequency distribution of different soil moisture contents. At high S values (close to ST) there will be a higher frequency of saturated conditions (and therefore higher potential to generate runoff), while at low S values the frequency of saturation will be low. Hughes and Sami (1994) also assumed that the spatial variability of S (expressed as the standard deviation of a Normal distribution around the mean value of S) would be lower during both dry and wet conditions and at a maximum at a mean sub-basin S of 0.75 * ST. The approach requires the definition of a maximum standard deviation (SDMAX) at the sub-basin moisture content of 0.75 * ST and the relationship used to calculate the standard deviation of the moisture content distribution (SD) for any value of S (Hughes and Sami, 1994) is:

for $S/ST > 0.75$

$$SD = (1.1 - S/ST) * SDMAX / (1.1 - 0.75) \dots\dots\dots 4.27$$

and for $S/ST \leq 0.75$

$$SD = (S + (0.75 - S/ST) * 0.2) * SDMAX / 0.75 \dots\dots\dots 4.28$$

Using the PDF, $N[S/ST, SD]$, it is possible to estimate the proportion of the sub-basin that contributes to runoff (Q/FT) for any value of S/ST as that part of the distribution that exceeds 0.9. The value 0.9 is assumed to be the threshold of relative moisture content at which interflow occurs. The relationship between

S/ST and Q/FT can therefore be used to estimate the POW parameter given that the Pitman model algorithm for runoff generation (Q) in any given month is:

$$Q/FT = (S/ST)^{POW} \dots\dots\dots 4.29$$

It has been assumed that lower values of SDMAX would be expected when there is little spatial variation in moisture content caused by slow moisture re-distribution processes after rainfall events (i.e. sub-basins with low topography and/or poorly drained soils), while higher values would be expected in steep topography with well drained soils. The approach is therefore based on estimating SDMAX using soil permeability and sub-basin slope, defining the S/ST versus Q/FT relationship and then finding an appropriate value of POW through a trial-and-error curve fitting approach (Kapangaziwiri, 2008; Kapangaziwiri and Hughes, 2008).

4.2.3.1 Estimating the maximum standard deviation of soil moisture content (SDMAX)

The estimation of SDMAX is based on values of sub-basin slope (BS) and soil permeability (K) and the derivation of their uncertainty distributions has been explained in previous sections. 5000 Monte Carlo samples are generated for each of BS and K and these are used to define samples of SDMAX based on the same classes used in Kapangaziwiri (2008) from which the PDF ($N[\mu_{SDMAX}, \sigma_{SDMAX}]$) of SDMAX is determined in the usual way.

The calculation of SDMAX is based on two components; a slope component (SL) and a permeability component (PERM). Table 4.3 explains how these components are calculated from classes of slope and permeability. The two components are then combined using:

$$SDMAX = 0.86 - 6 * (SL * PERM) / 100 \dots\dots\dots 4.30$$

The highest value of SDMAX is therefore 0.8 for well drained soils and steep slopes, while the lowest value is 0.32, corresponding to gentle slopes and poorly drained soils. Equation 4.30 as well as the classes and values given in Table 4.3 have been derived from experience with the use of this approach and have no real theoretical basis.

Table 4.3 Calculation of SL and PERM components as part of the estimation of SDMAX.

Slope component based on BS	SL value
$BS \leq 4\%$	3
$4\% < BS \leq 10\%$	2
$BS > 10\%$	1
Permeability component based on K (mm d^{-1})	PERM value
$K \leq 5$	3
$5 < K \leq 15$	2
$K > 15$	1

4.2.3.2 Estimating uncertain POW

The final approach to estimating POW has to account for both the variability in runoff from the soil component of unsaturated storage (ST_{soil}) and the deeper unsaturated zone (ST_{unsat}). 1000 samples are generated from each of the distributions of FT_{soil} , FT_{unsat} and SDMAX. The samples of the first two are combined to generate 1000 samples of the proportion of total interflow contributed by the two components (FT_{unsat} and FT_{soil}) of FT. The contribution of the unsaturated component is given by $FT_{\text{soil}}/(FT_{\text{unsat}} + FT_{\text{soil}})$ and that of the soil component is by $FT_{\text{unsat}}/(FT_{\text{unsat}} + FT_{\text{soil}})$.

For a range of S/ST values, equations 4.15 and 4.16 are used with the samples of SDMAX to construct a relationship between S/ST and $Q_{\text{soil}}/FT_{\text{soil}}$. This relationship is combined with an assumed relationship between S/ST and $Q_{\text{unsat}}/FT_{\text{unsat}}$ of the type:

$$Q_{\text{unsat}}/FT_{\text{unsat}} = (S/ST)^2 \dots\dots\dots 4.31$$

The relationships are combined using the weighting factors discussed above, such that for any value of S/ST the total interflow runoff (Q/FT) becomes:

$$Q/FT = (Q_{\text{soil}}/FT_{\text{soil}}) * FT_{\text{soil}}/(FT_{\text{unsat}} + FT_{\text{soil}}) + (Q_{\text{unsat}}/FT_{\text{unsat}}) * FT_{\text{unsat}}/(FT_{\text{unsat}} + FT_{\text{soil}}) \dots\dots\dots 4.32$$

An iterative procedure is used to find the value of POW that most closely matches this relationship using the Nash coefficient of efficiency as the objective function that has to be maximized. The above procedure generates 1000 samples of POW for each of the samples of FT_{soil} , FT_{unsat} and $SDMAX$, from which the mean, standard deviation, skewness and distribution type of POW are determined.

4.2.4 Estimating the infiltration parameters ZMIN, ZAVE and ZMAX

The infiltration parameters represent the spatially integrated process of infiltration. They control the absorption rate at the surface, the volume of water entering the moisture store reservoir and the volume of infiltration excess flow generated within a particular sub-basin. The parameters control the magnitude of the variable infiltration in the model, and effectively dictate the partitioning of rainfall into infiltration and surface runoff. Larger values of ZMIN and ZMAX increase the model infiltration and diminish the generation of direct runoff. A non-symmetrical triangular distribution of basin absorption, from a minimum of ZMIN to a maximum of ZMAX, is used in the model. ZAVE is the intermediate absorption rate of the distribution and determines the shape and symmetry of the triangular distribution. These parameters are assumed to be influenced by soil surface conditions and the characteristics of the basin average rainfall. The basis for the estimation approach is to use a variation of the physically based Kostiaikov (1932) infiltration equation to estimate a relationship between monthly rainfall depths and surface runoff. To achieve this, the monthly rainfall depths are approximately disaggregated using information about the expected rainfall characteristics of the sub-basin (e.g. mean number of raindays and typical rainstorm durations). The Pitman model infiltration function is then used to generate a similar surface runoff relationship using an iterative fitting procedure.

4.2.4.1 Estimating uncertain infiltration parameters

Basin monthly rainfall (m_{rain} , mm), maximum possible monthly rainfall (mm), number of rain days (r_{days} , days month⁻¹) and mean storm duration (r_{sd} , hrs) are required for the estimation of basin rainfall intensity given in mm h⁻¹. The monthly rainfall is disaggregated into daily rainfall using the number of rain days input variable and each day is then divided into 5 equal time periods, based on the mean storm duration, for which the rainfall intensities are calculated. These rainfall intensities are then compared with a frequency distribution of infiltration rates to generate an estimate of infiltration excess surface runoff. In this study,

the uncertainty has been incorporated through the variability within the infiltration rate parameters derived from the sub-basin soil properties. While it is recognized that there is also expected to be a great deal of uncertainty in the variables used to disaggregate the monthly rainfall, these were ignored in favour of computational simplicity. The basis of the calculation of the infiltration rates is a modified equation of the Kostiakov (1932) infiltration curve as used within the Variable Time Interval (VTI) model of Hughes and Sami (1994). The equation is expressed as follows:

$$\text{Infiltration rate (mm h}^{-1}\text{)} = B * C * T^{B-1} \dots\dots\dots 4.33$$

where T (mins) is the cumulative time from the commencement of the storm event and B and C are physically based constants whose mean values and their assumed spatial variability (expressed as the standard deviation of a log-Normal distribution) are estimated from soil texture properties and surface cover. B_{var} and C_{var} are used to define a log-Normal frequency distribution of infiltration rates at any given time T and the probability distributed principle of Moore (1985) is applied to determine the proportion of the sub-basin that contributes to infiltration excess runoff (Hughes and Sami, 1994). The spatial variability factors, B_{var} and C_{var} , are not however, estimated with uncertainty.

The constants of the infiltration equation are estimated with uncertainty to give an assumed Normal distribution of infiltration rates (IR) which can be expressed as:

$$N[\mu_{IR}, \sigma_{IR}] = N[\mu_B, \sigma_B] * N[\mu_C, \sigma_C] * T^M \dots\dots\dots 4.34$$

where $M = N[\mu_B, \sigma_B] - 1$.

The first step is to estimate the soil surface cover characteristics and their spatial variability for each of the terrain units i. The cover characteristics have been divided into 3 broad classes to simplify the process and default indices are used with these classes (Figure 4.7). The soil surface cover is taken to vary from well vegetated (index 0), through moderately vegetated (1) to crusting surfaces (2), while variability ranges from low (0), through moderate (1) to high (2).

Vegetation cover and variability for soil infiltration

Surface Cover - Top Slope: ☐ Well vegetated ☒ Moderately Vegetated ☐ Crusting

Cover variability - Top Slope: ☐ Low ☒ Moderate ☐ High

Surface Cover - Mid Slope: ☐ Well vegetated ☒ Moderately Vegetated ☐ Crusting

Cover variability - Mid Slope: ☐ Low ☒ Moderate ☐ High

Surface Cover - Bottom Slope: ☐ Well vegetated ☒ Moderately Vegetated ☐ Crusting

Cover variability - Bottom Slope: ☐ Low ☒ Moderate ☐ High

Accept Values Cancel

Figure 4.7 Screenshot of the classifications of soil surface cover and its variability that are used to determine the constants of the infiltration equation.

Estimating the PDF of infiltration constants B and C

The soil surface cover indices are summed across all the terrain units and then scaled to an integer that lies between 0 and 2. If the sum is greater than 2, then it is assumed to be 2. The estimate of the mean of the infiltration equation constant B is then calculated for each of the soil types in the basin. The estimation is based on a value of 0.79 for sands, 0.65 for sandy loams, 0.54 for sandy clay loams, 0.52 for sandy clays and 0.50 for clays. The texture based value is increased or decreased depending on the vegetation cover class scaling factor which would be either 0.2 (20%) or -0.2 for well vegetated or poorly vegetated (crusting) soils respectively. There is no scaling required for moderately vegetated soils. The effective scaled values for mean B across different soil types are given in Table 4.4.

Table 4.4 Values of the infiltration constant B for the different soil types and vegetation classes.

Soil type	Vegetation Cover		
	Well vegetated	Moderately vegetated	Crusting
sands	0.948	0.790	0.632
loamy sands	0.780	0.650	0.520
sandy clay loams	0.648	0.540	0.432
sandy clays	0.624	0.520	0.416
clays	0.600	0.500	0.400

The standard deviation of the distribution function of B is taken at a default 5% of the calculated mean value. Finally, 5000 Monte Carlo area weighted (based on

the proportion of the area of terrain unit i that is occupied by a soil type) samples are generated from which the mean, standard deviation, skewness and distribution type for constant B are determined.

The determination of the constant C is similar to that of B . The soil texture classes within a given basin are determined and the surface cover indices are summed across the terrain units to basin index, i.e. a summary description of the basin surface cover conditions. This index is used to determine the scaling factors for the soil types in the basin. These factors are 0.1 or -0.1 for well vegetated or crusting soils respectively, with no scaling required for the moderately vegetated class. The estimation is based on a value of 4.5 for sands, 3.5 for sandy loams, 2.5 for sandy clay loams, 2.0 for sandy clays and 1.0 for clays. The effective scaled values for the C values across different soil types are given in Table 4.5.

Table 4.5 Values of the infiltration constant C for the different soil types and vegetation classes.

	Vegetation Cover		
soil type	Well vegetated	Moderately vegetated	Crusting
sands	4.95	4.51	4.05
loamy sands	3.85	3.50	3.15
sandy clay loams	2.75	2.50	2.25
sandy clays	2.20	2.00	1.80
Clays	1.10	1.00	0.90

The standard deviation of the infiltration constant C is set at 5% of the calculated mean value. 5000 area weighted Monte Carlo samples generated from the distribution are used to determine the basin mean, standard deviation, skewness and distribution type for C .

Estimating the variability of infiltration B and C

The soil surface cover and cover variability indices are both summed across the terrain units to determine their sub-basin equivalents varying between 0 and 2. The matrices of the correction factors associated with B_{var} for the cover and the variability of this cover are (0, 0 and 0.25) and (-0.2, 0 and 0.2) respectively. These apply to the 3 classes of vegetation cover and variability shown in Figure 4.7. This implies that for surface cover there is no scaling deemed necessary for

the well and moderately vegetated classes whereas the crusting areas the values are scaled by 25%. For variability the values are scaled by 20% and -20% in well or poorly (crusting) vegetated soils with no scaling in moderately vegetated soils. The scaled values of B_{var} for both the cover and variability over different soil types are given in Table 4.6. The final value of B_{var} is an area weighted basin average summed across all the terrain units.

Table 4.6 Surface cover and variability factors used in the calculation of B_{var} based on the different vegetation cover and variability classes

	Vegetation Cover			Cover variability		
soil type	Well vegetated	Moderately vegetated	Crusting	High	Moderate	Low
Sands	0.008	0.008	0.010	0.015	0.012	0.010
loamy sands	0.018	0.018	0.022	0.022	0.019	0.015
sandy clay loams	0.012	0.012	0.015	0.022	0.019	0.015
sandy clays	0.012	0.012	0.015	0.015	0.012	0.010
Clays	0.008	0.008	0.010	0.015	0.012	0.010

The correction factors associated with C_{var} are (0.1, 0, and -0.1) and (-0.2, 0 and 0.2) related to the surface cover and its variability respectively. The factors across different cover and variability classes, used for the estimation of C_{var} are given in Table 4.7. The final value of C_{var} is an area weighted mean taken across all terrain units and soil types.

Table 4.7 Surface cover and variability factors across different soils used for the calculation of C_{var} .

	Vegetation Cover			Cover variability		
soil type	Well vegetated	Moderately vegetated	Crusting	High	Moderate	Low
sands	4.95	4.51	4.05	3.60	4.51	5.40
loamy sands	3.85	3.50	3.15	2.80	3.50	4.20
sandy clay loams	2.75	2.50	2.25	2.00	2.50	3.00
sandy clays	2.20	2.00	1.80	1.60	2.00	2.40
clays	1.10	1.00	0.90	0.80	1.00	1.20

4.2.4.2 Estimating uncertain ZMIN, ZAVE, ZMAX

The process explained in the preceding paragraphs generates PDFs of B and C parameters (defined by their mean and standard deviations) of the infiltration equation and their spatial variability, C_{var} and B_{var} . These are used to develop a relationship between monthly rainfall depths and total monthly infiltration excess runoff for each of 100 Monte Carlo samples taken from the distributions of B and C (independently). A simple water balance approach is also used in the approach to obtain an approximate estimate of the proportion of the sub-basin that is likely to be saturated and therefore will generate surface runoff for a given monthly rainfall value. This estimate is combined with the estimate of infiltration excess runoff to provide an estimate of total surface runoff for a given monthly rainfall total. An iterative process is then used for each sample of B and C to determine the best values of ZMIN, ZAVE and ZMAX that will reproduce the shape of the rainfall-surface runoff relationship (Figure 4.8) resulting in samples of these parameters. Note that at this point the parameter ZAVE is determined in relative terms only. The optimization is based on a simple objective function that minimizes the divergence between the two graphs up to a limit defined by an input variable defining the maximum expected monthly rainfall estimated from the rainfall time series. The outputs from this process are posterior distributions of ZMIN and ZMAX, while ZAVE (defining the skewness, or asymmetry, of the triangular distribution of absorption rates) is determined without uncertainty as the value that gives the best fit using the mean values of ZMIN and ZMAX. This final value of ZAVE is an absolute value. Figure 4.9 shows the uncertainty in the triangular shape of the infiltration process distribution as it is used in the estimation process. There are distributions around ZMIN and ZMAX while ZAVE is a fixed absolute value giving rise to the variation in the triangular distribution. Any combination of triangles between A-A and B-B together with ZAVE is feasible.

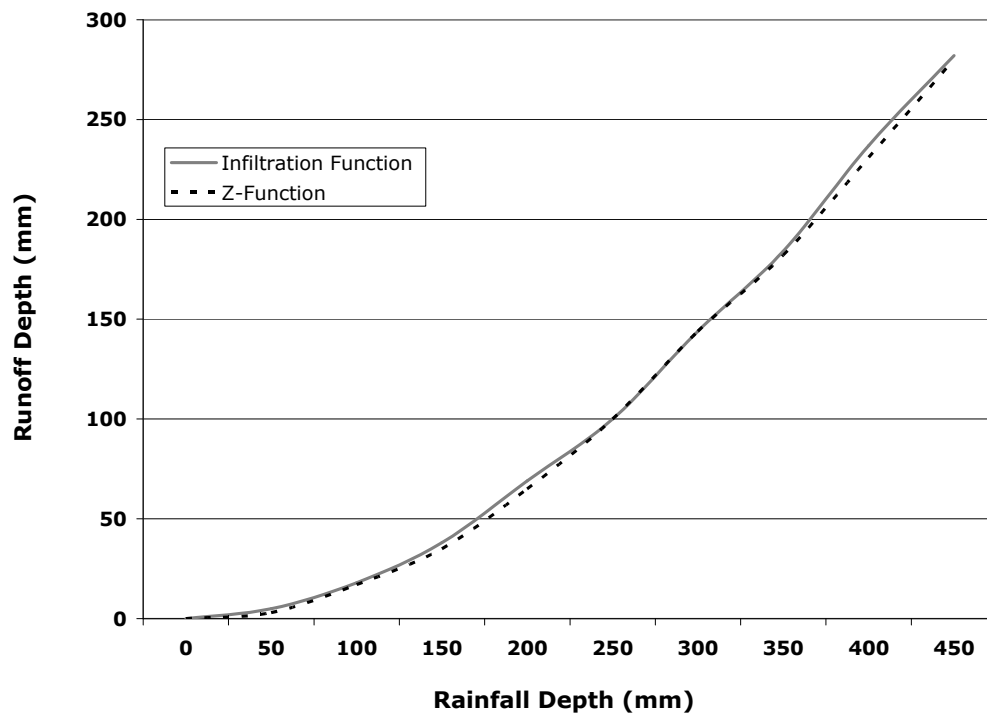


Figure 4.8 Graphs of runoff generated by the infiltration function and using the Pitman model function based on ZMIN, ZAVE and ZMAX

While the estimation procedure incorporates the concepts of both infiltration excess and saturation excess runoff, the Pitman model does not and in the model the surface runoff estimations are explicitly independent of moisture storage conditions. In developing the parameter estimation approach, the issue of saturation excess runoff could not be ignored and it is assumed that this is related to the difference in time scales used in the estimation procedure compared to the Pitman model algorithm. It is possible therefore that the Pitman model surface runoff algorithm is implicitly accounting for saturation excess runoff despite not being directly related to the simulated soil moisture level. It should also be noted that the values of the infiltration parameters are closely linked to the rainfall distribution factor that controls the way in which the total monthly rainfall is distributed over the four model iterations. Lower values of RDF will reduce the rainfall rate in the two main wet periods, while increasing it in the other two periods. Within a complete month the relationships between generated runoff, the RDF parameter and the infiltration parameters can be quite complex.

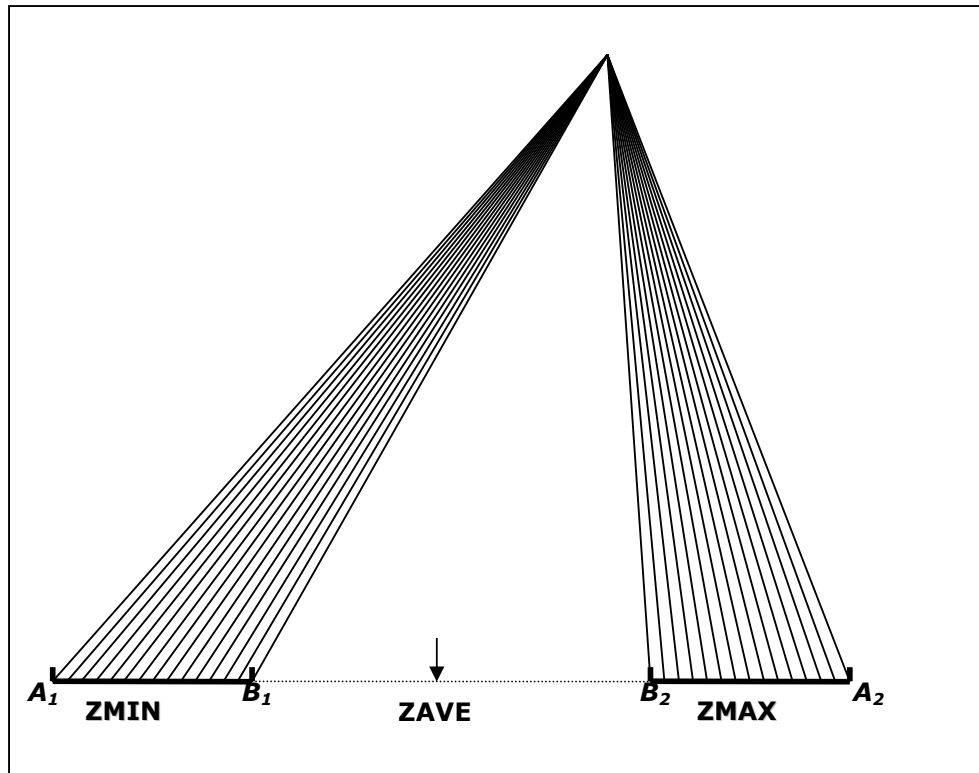


Figure 4.9 A diagrammatic representation of the uncertainty associated with the triangular distribution of basin absorption rates. A_1 - B_1 and B_2 - A_2 are the ranges of variability for ZMIN and ZMAX respectively. A-A and B-B represent the extremes of this representation.

4.2.5 Estimating uncertainty for the parameters PI1 and PI2

4.2.5.1 Establishing an estimation procedure for PI1 and PI2

The interception loss function depends on an interception capacity parameter (PI). The version of the model used in this study (Hughes, 2004; Hughes and Parsons, 2005) allows for this parameter to be seasonally variable and is determined for any two main vegetation regimes in a basin. The depth of rainfall intercepted in any month is based on an empirical relationship between the relevant PI parameter and rainfall depth, while interception storage satisfies the evaporation demand at the potential rate. The total interception loss (I mm/month) from any basin, based on empirical evidence, is estimated in the model by the algorithm (Pitman, 1973):

$$I = 13.08 * PI^{1.14} * [1 - e^{[p * (0.00099 * PI * 0.75 - 0.11)}] \dots\dots\dots 4.35$$

where p is the total precipitation depth for the month in mm and PI is the interception storage capacity of the vegetation given in mm.

The process of interception is affected by the percentage of the ground covered by the vegetation and the leaf area index (LAI) of the vegetation type (Rutter et al., 1975). Both of these can depend upon the stage of development of the vegetal cover and the season of the year. It should also be noted that at the basin scale there will almost always be large spatial variations in interception capacity. There are a number of literature sources that have documented interception losses for different vegetation types (for example, Rutter et al., 1975; Schulze, 1995; Hall, 2003). A direct comparison between the parameter values and measured interception capacity is somewhat confused by the model assumption that the stored water evaporates completely in a single day. In reality, within a monthly time step model, the extent to which this assumption can be considered valid will depend upon the typical patterns and distribution of rainfall within a month. If the total monthly rain falls in concentrated periods of several days it is likely that the model will over-estimate interception losses.

The approach that was therefore taken to estimate the interception parameters is an empirical one. The principle is to develop a relationship between the model parameter PI and interception loss based on vegetation attribute data. To achieve this, it is necessary to generate the losses at the smallest possible temporal scale so that the variations of the interception process can be accounted for. However, the aim of the estimation procedures is to use data that are accessible within the region with relative ease and rainfall records at a scale of less than a day are not very common. Therefore, daily rainfall records were used. The VTI (Variable Time Interval, Hughes and Sami, 1994) model uses physically-based algorithms for the determination of daily interception loss from rainfall data which are based on the method of Rutter et al. (1975). This depends on the vegetation characteristics defined for five default cover classes based on an understanding of vegetation types that occur within the region. These are dense forest, bush/sparse forest, dense crop/groundcover, sparse crop/groundcover and bare soil and estimates of these (and their seasonal variation) are primary inputs for the parameter estimation procedures (see Figure 4.5). Related to these, and used in the model, are the proportion of vegetation cover, the leaf area index and the vegetation

canopy capacity. These properties are estimated using the proportion of the basin covered by the five broad vegetation cover classes. Default LAI values associated with each of the cover classes are used in the estimation process and these are shown in Table 4.8. The LAI values are broadly in agreement with the values reported for similar vegetation classes in the literature (for example Scurlock et al., 2001).

Table 4.8 Default LAI values for different vegetation cover classes that are typical in the region

Vegetation type	LAI
Dense Forest	5.0
Bush/Sparse forest	3.0
Dense crop/groundcover	1.5
Sparse crop/groundcover	0.5
Bare soil	0.0

Mean monthly interception losses from daily rainfall records were calculated using the VTI (Hughes and Sami, 1994) model. The Pitman (Pitman, 1973) model parameter PI was manually adjusted until a similar magnitude of loss was achieved by the monthly model. This process was carried out for some 20 basins selected to represent the hydro-climatic and physiographic conditions prevailing in South Africa. Based on the results from these selected basins, relationships between rainfall, interception loss and the interception capacity parameter (PI) were explored and developed. The effect of the frequency of rainfall was considered important and the average number of raindays was included as a predictor variable. Figure 4.10 shows the relationship between the monthly interception losses (generated by the VTI model based on daily records), the average percentage of the number of rain days per year (NRD) and mean annual precipitation (MAP) at different values of calculated LAI determined by different combinations of vegetation types.

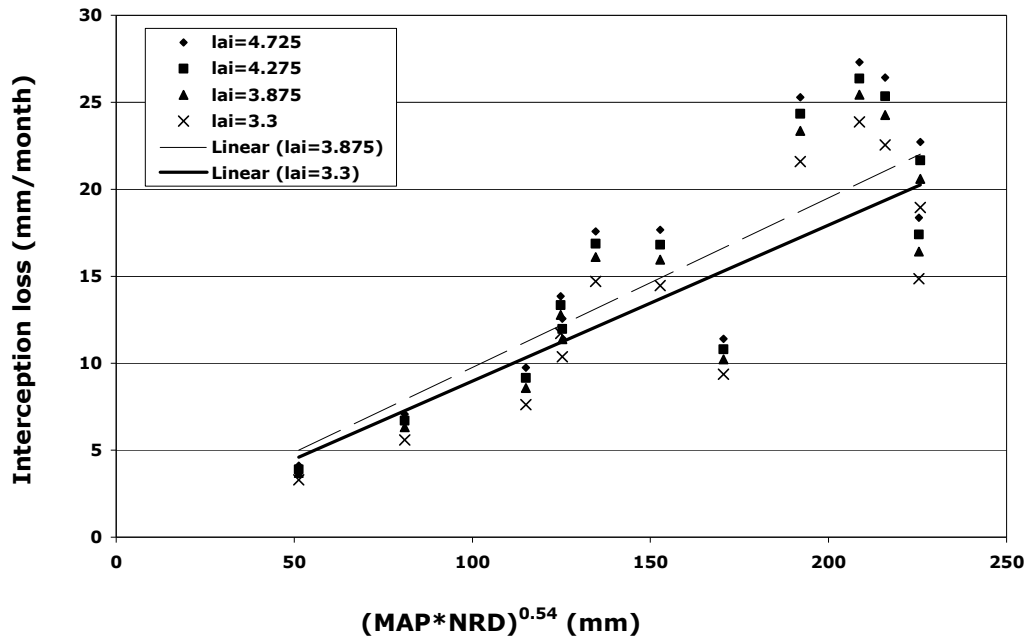


Figure 4.10 The relationship between VTI generated interception loss and MAP and NRD at different values of LAI.

After a number of exploratory tests with different equation formats, it was decided to use a power function (equation 4.36) with a fixed exponent and a gradient (Grad1) that is a function of LAI (equations 4.37 and 4.38):

$$\text{Interception Loss} = \text{Grad1} * (\text{MAP} * \text{NRD})^{0.54} \dots\dots\dots 4.36$$

From an investigation of the variation of the most appropriate Grad1 value with LAI it was realised that there was a distinct differences for LAI values below than and above an LAI of approximately 1.8. Grad1 has therefore been assumed to vary linearly with LAI when greater than 1.8, while an 'S' curve relationship using the hyperbolic tangent function was appropriate for LAI values less than 1.8. These relationships are written as:

for LAI > 1.8

$$\text{Grad1} = 0.1124 * \text{LAI} + 0.4481 \dots\dots\dots 4.37$$

and for for LAI < 1.8

$$\text{Grad1} = 0.65 * [\text{Tanh} \{1.2 * (\text{LAI} - 1.8)\} + 1.0] \dots\dots\dots 4.38$$

Using monthly data for the selected basin and the algorithms of the Pitman (Pitman, 1973) model, the PI parameter was adjusted to generate equivalent monthly interception losses to those determined by the VTI model. The values of monthly interception loss were plotted against MAP for different values of PI as shown in Figure 4.11.

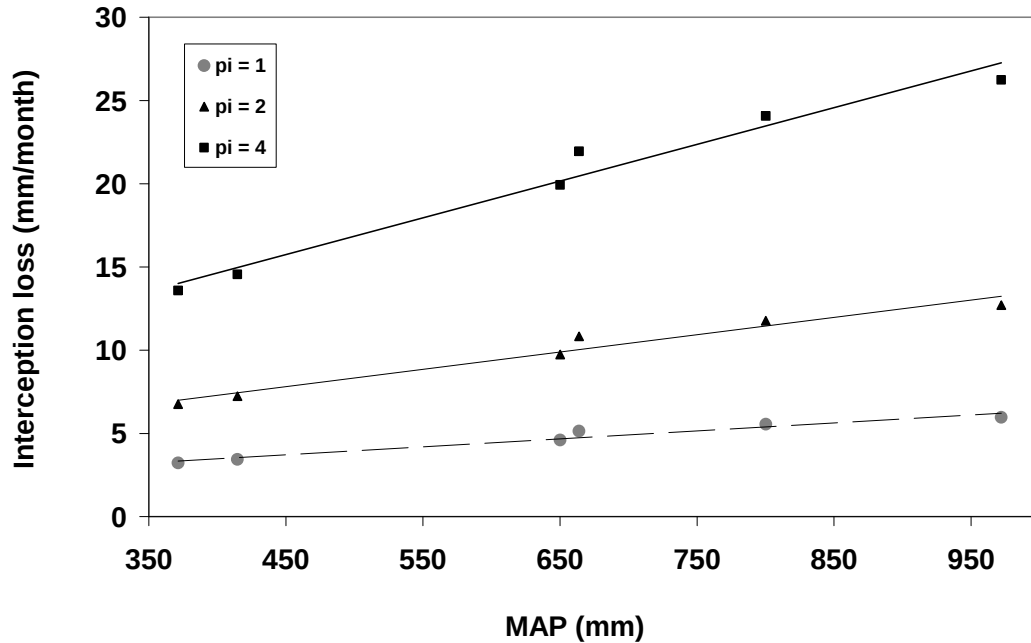


Figure 4.11 The relationship between MAP and Pitman interception loss (equivalent to VTI interception loss) at different values of parameter PI.

For the different values of PI, the following relationship between MAP and interception loss was established:

$$\text{Interception loss} = \text{Grad2} * \text{MAP} \dots\dots\dots 4.39$$

where Grad2 is the gradient. PI values that generate the same interception loss values used in the equation 4.39 were used to establish a relationship between PI and Grad2 (Figure 4.12):

$$\text{PI} = 133.38 * \text{Grad2} \dots\dots\dots 4.40$$

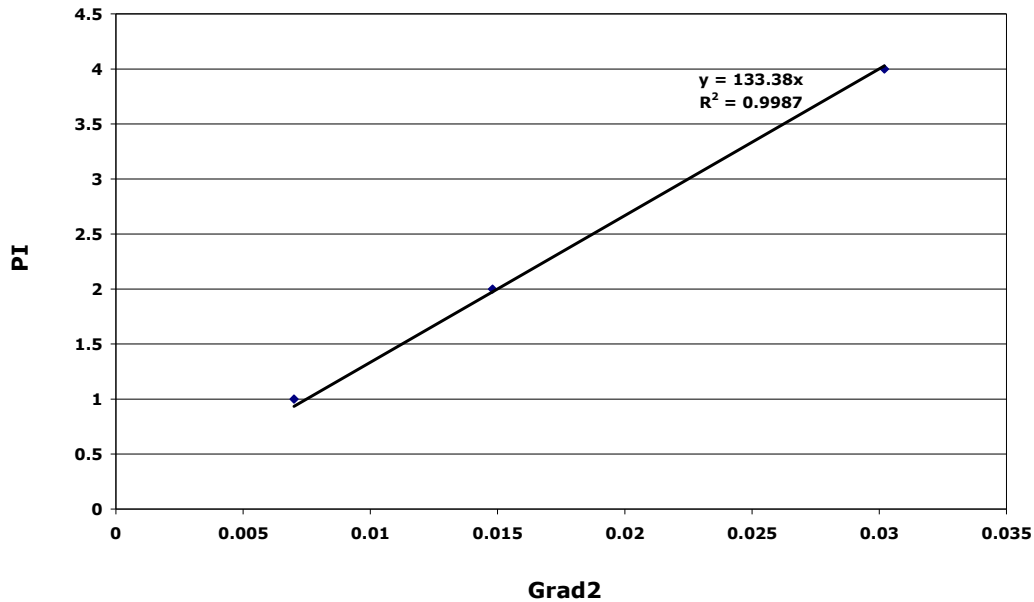


Figure 4.12 The relationship between parameter PI and gradient of the relationship between MAP and monthly interception loss using the Pitman model algorithms.

Thus based on monthly data and the Pitman model algorithms, the estimation equation for the parameter PI was determined as follows:

$$PI = 133.38 * \text{Interception loss} / \text{MAP} \dots\dots\dots 4.41$$

where monthly interception loss is estimated using equations 4.36 to 4.38.

This procedure is repeated four times to account for the seasonal estimations (i.e. summer and winter) for each of the two dominant vegetation types (i.e. vegetation 1 and vegetation 2) in a basin resulting in estimates for PI1s, PI1w, PI2s and PI2w.

4.2.5.2 Estimating uncertain PI1 and PI2

The incorporation of uncertainty into the estimation procedures for the interception parameters is based on the variability in the estimates of the proportion of the basin under a given vegetation cover class (a primary input) to estimate the uncertainty in the determination of LAI. The distribution of the interception parameter PI is therefore given as:

$$N[\mu_{PI}, \sigma_{PI}] = \{133.28 * N[\mu_L, \sigma_L]\} / MAP \dots\dots\dots 4.42$$

where L is the monthly interception loss whose distribution is determined from:

$$N[\mu_{IL}, \sigma_{IL}] = N[\mu_{Grad1}, \sigma_{Grad1}] * (MAP * NRD)^{0.54} \dots\dots\dots 4.43$$

and the uncertainty in the estimation of the gradient of the VTI interception loss is given by:

for LAI > 1.8

$$N[\mu_{Grad1}, \sigma_{Grad1}] = 0.1124 * N[\mu_{LAI}, \sigma_{LAI}] + 0.4481 \dots\dots\dots 4.44$$

and for LAI < 1.8

$$N[\mu_{Grad1}, \sigma_{Grad1}] = 0.65 * [\text{Tanh}\{1.2 * (N[\mu_{LAI}, \sigma_{LAI}] - 1.8)\} + 1.0] \dots\dots\dots 4.45$$

The primary input of the proportion of the basin under a particular vegetation cover class is estimated from a number of possible vegetation types. Default estimates for the proportions of the vegetation type classes are provided in the parameter estimation software for a series of typical vegetation regimes found in the region (Figure 4.13 and Table 4.9). The variability in the proportion of basin covered by any given vegetation cover class is specified as a range from the minimum to the maximum. The seasonal variation is accounted for through the specification of basin proportion ranges for both winter and summer seasons. The default values that have been built into the estimation equations can be changed should there exist better knowledge about variations of vegetation cover in a basin. It should also be noted that the secondary vegetation in Figure 4.13 was assumed to be a land use change to afforestation which is the typical situation in South African catchments. It was deemed to include this since this is a typical water resource problem in the country.

Figure 4.13 The vegetation classes typically found in the region that are used for the estimation of vegetation interception parameters.

For each vegetation cover class i , a normal distribution function of proportions of basin area under a given vegetation cover class (vc_i), defined by μ_{vc_i} and σ_{vc_i} , is determined from the primary input data as follows:

$$\mu_{vc_i} = (H_i + L_i) / 2 \dots\dots\dots 4.46$$

and

$$\sigma_{vc_i} = \text{abs} (H_i - L_i) / 3.3 \dots\dots\dots 4.47$$

where H_i and L_i are the high and low estimates of proportion of the basin under vegetation cover class i . The assumption made for the determination of the standard deviation is that the low and high cover estimates encompass 99% of all the values of a cumulative normal distribution of basin proportions under vegetation cover classes. This assumption implies that these extreme values represent 3.3 standard deviations from the mean value. Absolute values are used in the standard deviation estimate (equation 4.47) to avoid negative values that will arise in situations where a 'high' estimate is smaller than the 'low' one.

Table 4.9 Example of the default values of vegetation cover ranges used to estimate LAI and other vegetation parameters. Est refers to estimate.

Vegetation type	Summer		Winter	
	Low Est	High Est	Low Est	High Est
Dense indigenous forest				
Dense Forest	0.80	0.90	0.80	0.90
Bush/Sparse forest	0.20	0.10	0.20	0.10
Dense crop/groundcover	0.00	0.00	0.00	0.00
Sparse crop/groundcover	0.00	0.00	0.00	0.00
Bare soil	0.00	0.00	0.00	0.00
Mixed indigenous forest and grazing land				
Dense Forest	0.40	0.50	0.40	0.50
Bush/Sparse forest	0.10	0.20	0.10	0.20
Dense crop/groundcover	0.50	0.30	0.50	0.30
Sparse crop/groundcover	0.00	0.00	0.00	0.00
Bare soil	0.00	0.00	0.00	0.00
Dense bush and grassland				
Dense Forest	0.00	0.00	0.00	0.00
Bush/Sparse forest	0.60	0.70	0.60	0.70
Dense crop/groundcover	0.30	0.30	0.30	0.30
Sparse crop/groundcover	0.10	0.00	0.10	0.00
Bare soil	0.00	0.00	0.00	0.00
Mixed grassland and cultivation				
Dense Forest	0.00	0.00	0.00	0.00
Bush/Sparse forest	0.00	0.00	0.00	0.00
Dense crop/groundcover	0.50	0.60	0.50	0.60
Sparse crop/groundcover	0.30	0.30	0.30	0.30
Bare soil	0.20	0.10	0.20	0.10
Arid bush, groundcover & bare soil				
Dense Forest	0.00	0.00	0.00	0.00
Bush/Sparse forest	0.10	0.10	0.10	0.10
Dense crop/groundcover	0.15	0.20	0.15	0.20
Sparse crop/groundcover	0.55	0.60	0.55	0.60
Bare soil	0.20	0.10	0.20	0.10

5000 Monte Carlo samples are generated from the distributions of each vegetation cover class i . Each sample is summed across the different vegetation cover classes and the result is multiplied by LAI_i , the value of the leaf area index

associated with that vegetation cover class i resulting in 5000 samples of LAI for the basin dominant vegetation type. From these samples the basin mean, standard deviation, skewness and distribution type for LAI are calculated. The process is repeated 4 times for the determination of the summer and winter LAI distributions for each of the two vegetation types in the basin.

4.2.6 Estimating the groundwater recharge parameter GW

4.2.6.1 Introduction

It has been assumed that the maximum recharge rate (GW mm month^{-1}) from the moisture store is influenced by the same factors affecting FT, including soil texture and structure. However, while topography will play a major role in the determination of FT (slope gradients in areas with low topography will be insufficient to generate much lateral drainage), it will play a lesser role in the vertical recharge process. The information typically available to define the vertical structure of the unsaturated zone and its relationship with surface topography is rarely detailed.

The Pitman model uses the following algorithm to calculate monthly estimates of groundwater recharge depth (Q_{rech} mm):

$$Q_{\text{rech}} = \text{GW} * [(S - \text{SL})/(\text{ST} - \text{SL})]^{\text{GPOW}} \dots\dots\dots 4.48$$

where S , ST and SL are the current basin mean moisture content (mm), the moisture content at basin saturation (mm) and the lower limit of soil moisture (mm) below which no recharge is possible respectively. SL is normally set to zero without compromising the results since rates of recharge at low soil moisture are small and have little influence on the total water balance of the basin (Hughes and Parsons, 2005). In the estimation process the GRAII values of mean annual recharge (MAQ_{rech}) are used with a simple moisture balance approach. A number of sub-basins (15) for which calibrated parameter values were available were used to determine a relationship between the appropriate value of S to use in equation 4.24 to generate mean monthly recharge ($\text{MMQ}_{\text{rech}} = \text{MAQ}_{\text{rech}}/12$).

$$S = 0.26 * \{P - \text{ET} - (\text{FT}/\text{POW}) - \text{MMQ}_{\text{rech}}\}/\text{ST} + 0.54 \dots\dots\dots 4.49$$

where P and ET are mean monthly rainfall and potential evaporation, both in mm.

The mean values of parameters ST, FT and POW are used and it has been assumed that SL is always 0, while GPOW has been set to a constant value of 3. It was found to be difficult to determine values for the two constants in equation 4.25 (0.26 and 0.54) that could be considered appropriate to sub-basins drawn from different physical and climate settings. However, attempts to include additional variables within equation 4.25 did not improve the situation and it is acknowledged that the estimation equation for GW is less than satisfactory and needs to be improved at a later stage.

4.2.6.2 Estimating uncertain GW

To estimate uncertainty related to the estimation of GW implies the specification of a PDF for the parameter which is based on the uncertainty in the estimation of the mean basin moisture content, S. The uncertainty in the estimation of S will then be influenced by the distributions of ST and FT (POW is taken with no uncertainty) and is expressed as:

$$N[\mu_S, \sigma_S] = 0.26 * \{P-ET-(N[\mu_{FT}, \sigma_{FT}]/POW) - N[\mu_{MMQ_{rech}}, \sigma_{MMQ_{rech}}]\} / N[\mu_{ST}, \sigma_{ST}] + 0.54 \dots\dots\dots 4.50$$

The determination of the distributions of ST and FT were discussed in earlier sections and will not be repeated here.

Determining the mean and standard deviation of Q_{Rech}

Two values of mean annual groundwater recharge estimates, taken from the GRAII national database, representing the upper (U) and lower (L) limits of mean annual recharge are used to estimate the distribution properties (assuming a Normal distribution) of mean monthly recharge:

$$\mu_{MMQ_{rech}} = (U + L) / 24 \dots\dots\dots 4.51$$

$$\text{and } \sigma_{MMQ_{rech}} = (U - L) / (12 * 2.33) \dots\dots\dots 4.52$$

The calculation of $\sigma_{MMQ_{rech}}$ is based on the assumption that the limits, U and L, represent the 1st and 99th percentiles (i.e. 2.33 standard deviations about the mean) of the cumulative Normal distribution function of MMQ_{rech} .

1250 samples are generated from each of the distributions of ST, FT and MMQ_{rech} and are used to estimate different soil moisture states, S which are used in

equation 4.24 to generate the samples of GW and therefore the distribution characteristics of this parameter.

4.3 Summary Remarks

This work has focussed on the estimation of the uncertainty for the parameters described in this chapter. It is conceded that there will be uncertainties related to the other parameters not considered here. The work on parameter uncertainty will proceed beyond the time limits of this PhD project and the work reported here is used as a preliminary assessment of the methods that are applicable given the type of information available in the country. Where it is necessary to include uncertainty in other parameters, it is recommended that a uniform distribution is used and the maximum and minimum values are set to feasible ranges of the parameter values.

Of the parameters that were not dealt with in this study, R (with values between 0 and 1), which describes the relationship between soil moisture and evaporation, is likely to have a significant influence on the runoff generation processes. It is envisaged that its estimation with uncertainty is likely to increase overall uncertainty propagated through the model. The estimation of this parameter would require information on vegetation characteristics related especially to rooting depth and density and it was found to be difficult to access useful information of this type for the region. In the current study, uncertainty in parameter R is estimated using a uniform distribution based on our understanding of the conceptual physical meaning of the parameter (Kapangaziwiri, 2008). R is expected to be higher (i.e. closer to 1) in more arid and less densely vegetated areas and lower in more humid and well vegetated areas. In this study therefore, the minimum and maximum values are set arbitrarily between 0 and 0.3 for wet basins, 0.3 and 0.7 for sub-humid/semi-arid basins and 0.7 and 1 for arid basins.

While the incorporation of uncertainties in the parameter estimation process is important for water resources estimation, it is recognized that the application of the methods discussed in this section are subject to several sources of inconsistency. The methods suggested for estimating uncertainty are designed to account for the differences in scale between the basin property data and the model. However, there remains a degree of subjectivity in the interpretation of the physical data. This is particularly relevant to regions where there is a large degree of variability in the AGIS (2007) land type data within a single model sub-

basin. In these situations, the process of selecting the relevant values for the parameter estimation process becomes quite complex. In other parts of the southern African region, where the same type of basin property data do not exist, the available data would require different interpretation approaches. This will inevitably introduce further subjectivity. The estimation equations themselves, while considered to be conceptually credible, are generalizations of known hydrological principles. They are therefore subject to essentially unknown structural uncertainties. However, in spite of these potential sources of subjectivity, the method is expected to generate more consistent parameter sets than those based on calibration and regionalization. The basis for the different number of Monte Carlo samples used (1000, 1250, 1500, 2000 and 5000 were used) has mostly been pragmatic depending on the calculations, with a smaller number being used to reduce computing time where the estimation process is iterative. Different percentiles were also used for the normal distribution as well as different default values of the standard deviation in proportion to the mean. This was based on how extreme the sample values are considered to be.

A relevant overall conclusion at this point is that while the parameter estimation process has been significantly improved, there is still some work required in some areas. The most significant area relates to the interpretation of the AGIS (2007) land type information, especially the soil depth and texture data. This problem is closely related to the issue of scale. There will always be subjective interpretation of the land type information in cases when a number of land types (and therefore soil types) occur in the same sub-basin. The ensuing process of lumping is expected to affect the parameter estimation process and therefore the model outputs. One of the main questions that arise is therefore whether a reduction in the scale of modelling, and therefore a reduction in the scale of parameter estimation, is likely to be rewarded with improved results. This improvement might be evaluated by better correspondence with observed data in gauged basins and a reduction in uncertainty in ungauged basins.

It is important to recognize that the *a priori* parameter estimation process is only one part of the overall uncertainty framework (discussed in Chapter 3 and illustrated in Figure 3.3). In the context of this framework, the output uncertainty resulting from the *a priori* parameters is further assessed using the regional constraints (Chapter 5). This is the importance of the feedback loop proposed in the application framework (Figure 3.3).

CHAPTER 5

DEVELOPMENT OF CONSTRAINTS

5.1 Introduction

It was established in Chapters 2 and 3 that making predictions in ungauged basins necessitates a change in the mindset of hydrological model applications. The traditional approach that relies on calibration does not work in many basins of the world and especially in southern Africa where the density of runoff measurement networks are low. This means that the classical methods of regionalization are of little use. The unfortunate problem has been that while there has been phenomenal growth in the sophistication of hydrological models over the past few decades (mainly due to technological improvements in computing power) little has been done about collecting additional data. While there are remote sensing data collection platforms, these have not been used much and confidence in their use will grow with longer periods of overlap with historic ground-based observations that should be used to 'calibrate' these data (so called ground-truthing). Therefore, the role of observed data is critical (Silberstein, 2006) and cannot be over-emphasized. It is argued that modelling in the absence of adequate data is not science, unless it is to develop hypotheses that are to be tested by observation and that improvement in the management of our environment and water resources will not come with improved models in the absence of improved data collection because we cannot manage what we do not measure. Seibert and MacDonnell (2002) advocate the use of 'soft data' to condition model process representation and, consequently, improve predictions. The use of hydrological response characteristics, while not strictly soft data, is gaining importance in conditioning and constraining hydrological models especially in ungauged basins.

One of the PUB approaches has been to explore the use of physical basin characteristics to either estimate parameter variation across different places (*a priori* parameter estimation) or to explain hydrologic behaviour of catchments. Both of these initiatives are explored in this study within an uncertainty framework, with the former discussed in chapter 4. The latter forms the basis of this chapter. The physical characteristics are used to aid the identification of consistent and hydrologically plausible models in a manner that is akin to the calibration process. This is achieved through the use of basin characteristics

related to hydrological signatures. The underlying principle is that physical basin characteristics (through hydrological signatures) can be used as surrogates, or are large scale markers of intrinsic local scale hydrological processes. While this is nothing new and has long been recognized and implicitly accepted, explicit quantification of these relationships is relatively new and is still an open problem. Thus, when dealing with ungauged basins, it is more prudent and scientifically sound to look for hydrological signatures (usually defined by basin physical or climatic characteristics) of the processes being simulated instead of insisting on just modelling exercises and model testing. In fact, looking for hydrological signatures, and basing our hydrological predictions on these, may open new avenues of research that are capable of providing answers to problems about uncertainty in hydrological predictions. Thus, if relationships between basin characteristics and hydrological signatures can be defined, this would make regionalization of models and model application in ungauged basins more consistent and objective. And, if statistical confidence and/or prediction boundaries around these relationships can be included then the uncertainty related to model predictions can also be quantified and analysed (Figure 5.1). While this is a nontrivial issue, it is a hydrologically plausible and scientifically sound alternative to calibration and regionalization.

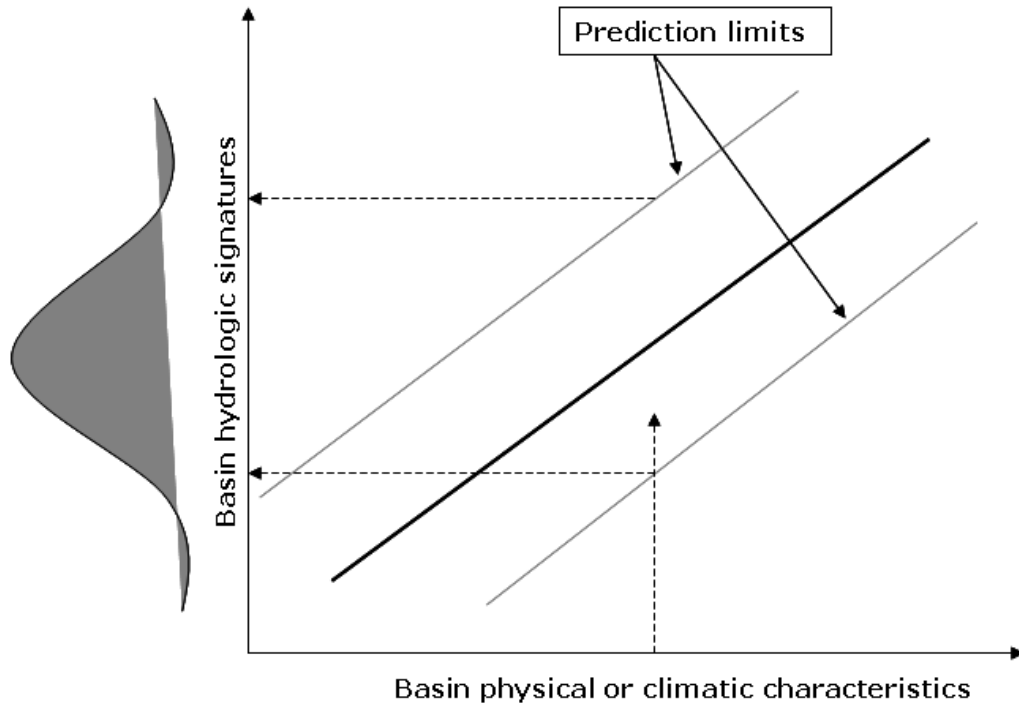


Figure 5.1 The uncertainty related to hydrological signatures based on relationships with basin characteristics

In the context of the framework discussed in Chapter 3, a hydrological signature is defined as an index of the time series of a basin's dynamic response characteristics (e.g. runoff coefficient) and reflects the basin's functional behaviour (Wagener et al., 2007, Yadav et al., 2007). Such indices of catchment behaviour are capable of being regionalised using simple regression relationships whose prediction limits are used to define the distribution of possible 'behaviour'. Indices are often used as model diagnostic tools to constrain and condition continuous flow simulations at both gauged and ungauged sites. Signatures are pattern extracts of the input-state-output behaviour of a real system (representing the functional characteristics of the system) while the indices that are derived from the signatures are pattern properties of the same system (Gupta et al., 2008). Applied properly (i.e. with all the uncertainties reduced considerably) they are better than calibration whose focus is on the goodness of fit between observations and simulations (Vogel and Sankarasubramanian, 2003). They can therefore be important in separating the consistent (i.e. behavioural) model outputs from those that are not. Indices are often loosely referred to as just constraints, because they can be used to constraint all possible model output results.

Constraints are derived from output or input-output time series measured within the basin, including precipitation, evapotranspiration, streamflow or any other response variables (Yadav et al., 2007). Such response characteristics are often indicative of how a given basin differs from others and examples include common descriptors of hydrograph shape such as runoff ratio, slope of the recession curve and time to peak flow (Shamir et al., 2005). The major advantage with constraints is that they are hydrological fingerprints of catchment behaviour and are thus model independent. The approach adopted in this study provides for the generation of ensemble predictions in ungauged basins and the use of regionalized basin functional characteristics (or indices) to constrain ensembles of model predictions. The objective is to achieve a progressive reduction in predictive uncertainty by constraining model output to expected watershed behavior at both gauged and ungauged locations, while maintaining reliable and/or consistent predictions (Yadav et al., 2007).

5.2 Development of constraints for South Africa

In the context of the framework, regional constraints are regional priors on the expected catchment hydrologic responses. In ungauged basins, these are

equivalent to historical observed information in traditional model calibration. The basic assessment of hydrological model simulations has been achieved through the hydrograph and in gauged basins the simulated flows are compared with the observed flows. It is contended here that if the use of constraints is to be successful then the choice of constraints for use in any region should encompass as many aspects of the hydrograph as possible. This ensures an all round assessment of the hydrological system under investigation. The other important considerations when selecting constraints are:

Data availability and quality: For reliability and consistency the construction of constraints must be based on reliable information about observed natural hydrological system response. This implies that many of the available historical observed streamflow records are not suitable for this purpose. Besides the effects of abstractions, impoundments, diversions and land use changes, these records are also subject to measurement error and flow levels beyond the instrument limits are often estimated based on extrapolation equations. The applicability of these equations beyond the measurement limits is a contentious issue. During critical flood conditions extrapolation equations are highly uncertain and resultant high flow records need to be used with caution. Some pre-processing, to naturalize the flows (i.e. remove non-natural effects) may be necessary; however, these approaches are unfortunately subject to uncertainty. This compromises the quality (accuracy and representativeness) and usefulness of the constraints based on these data.

Hydrologic relevance: constraint indices must be hydrologically relevant and measure some property of the hydrological response characteristics.

Capable of extraction from the simulated flows: If a constraint index cannot be estimated from the model output so that it can be compared against its equivalent based on observed information, then it ceases to be useful. The whole purpose of using constraint indices is to be able to guide model applications by restricting the simulated responses to within the range of likely or behavioural (Beven and Binley, 1992) responses determined from the observed data.

Suitable predictors: Constraints are a representation of a basin's functional characteristics and their construction is dependent on the availability of suitable basin physical and/or climatic information. These are known as predictor variables and must be available at suitable scales (spatial and temporal) and with minimum

uncertainty. As discussed in Chapter 2 uncertainty ranges are often defined by a 95% confidence interval when sufficient information about the distribution is at hand. The 95% prediction limits of the regression relationships used to estimate the regional constraints can be used to define the extent of their uncertainty. If these limits are too wide as a consequence of the choice of unsuitable predictor variables, they will fail to effectively condition model outputs.

South Africa has had a long history, since the 1970s, of water resources assessments with the 1990 project (WR90, Midgley et al., 1994) being the most popular and the 2005 project (WR2005, Bailey, 2009) being the most recent update of all the previous assessments. This has created a huge database of hydrological data and conventional wisdom on water resources of the country. These data, and a reasonable network of river flow observation gauges, are invaluable in the quest to develop constraints that would allow the application of hydrological modelling in ungauged basins. While the gauge network is reasonable, the extent to which the observed data are representative of natural hydrology conditions is dubious given unquantified upstream human influences. A number of possible constraint indices and their predictor variables were thus investigated before three relatively simple ones were chosen for development and testing. Therefore, while other indices are still being considered, as the project develops further, only three are reported in this study. These are the mean annual runoff ratio, slope of the monthly flow duration curve and mean annual ground water recharge. The choice and subsequent development of these constraints is driven by the quest to answer the question relating to how to diagnose the hydrology (at a given temporal scale) of any basin based on observed surface runoff and relevant climatic and physical data.

5.2.1 Mean annual runoff ratio (Q/P)

This constraint is used to describe the overall water balance of a basin and is an indication of how well the model is simulating the water balance of the basin given the input information. The development of the constraint is based on the concepts of Budyko (1974) using a measure of aridity to predict expected runoff. This is achieved using regionalized relationships of Q/P against P/PE, where Q is runoff, P rainfall and PE is potential evapotranspiration.

Development of the constraint relationships

In South Africa the series of water resources estimation projects has resulted in country-wide estimates of hydrological information. The country is divided into 1946 so called 'quaternary catchments' for which simulated (and in some cases observed) data on hydrological variables are available. The current database, so called WR2005 (Bailey, 2009) which used data up to the 2004/2005 hydrological year, had not been released at the time of the development of these relationships. The relationships are therefore based on the WR90 data (Midgley et al., 1994), that is based on data from 1920/1921 up to 1989/1990 hydrological years. The first step was intended to cover the whole country and therefore used the simulated mean annual runoff (Q) from the 70 year (1920 to 1990) WR90 runoff time series and the estimated mean annual rainfall (P) and potential evaporation (PE) for all 1946 quaternary catchments (Midgley et al., 1994). The runoff data used were the incremental flows, which are flows generated only within each quaternary catchment. The objective of initially using the simulated flows was to achieve total coverage of the country and to try and identify different regions of similar response relationships. A scatter plot of all these data suggested a series of log-log relationships that converge at low values of both P/PE and Q/P. An iterative process was followed to define five regional relationships. The relationship for the first region, Region 1, was first established by identifying a regression equation that had a high R^2 value and for which the residuals were approximately equally divided between negative and positive values. Once the points to be included in Region 1 were finalised, the same process was followed to identify the Region 2 points and so on. All of the points and the resulting regression relationships are shown in Figure 5.2, while Table 5.1 lists the equations and the relevant R^2 values. Note that in Figure 5.2 (and also Figure 5.3) Q/P values above 1 would be results of data errors in either Q or P estimates, e.g. significant over-estimation of flow or significant under-estimations of rainfall. Figure 5.4 indicates that the regions are generally spatially contiguous although there are some areas that are not clearly defined as a single region. This may be due to localised variations in runoff response, as well as artefacts related to errors in the data and the use of simulated data.

In spite of the reasonably good results resulting from this process, it would not be strictly good scientific practice to develop the regional constraint relationships based on simulated data, although it is considered to be acceptable to use these data to initially define the regions. However, these are the only data that have a reasonable national coverage and were therefore deemed a good starting point

for a first order definition of regions before these regions can be refined using the more spatially limited naturalised observed flow data for a final definition of the relationships. Therefore, the second step involved the use of the naturalised observed time series (also given in Midgley et al., 1994) for all available stream flow gauges. These data required some filtering and quality checks before they could be used. Gauges were initially rejected if they had less than 10 years of observations, if their drainage areas included quaternary catchments that fell into more than a single region or if the amount of missing (and in-filled) data was excessive. Some very small gauged sub-basins were also rejected as they were not expected to be representative of quaternary catchment scale responses. This process reduced the number of gauges to 270 within the whole country. The spatial coverage of these gauges was such that some regions are better represented than others which could impact on the relationships (Table 5.1). However, given that the initial regions were based on all quaternary catchments the reasoning was that the effects should not be too severe. If the relationships for the gauged basins were not too different from the ones based on simulated data, then it was hypothesised that the spatial distribution of the gauges is not a critical consideration. For each of the regions identified during the first step, Table 5.1 lists the number of gauges included in the analysis, the range of catchment areas, the coefficients of the final estimation equations and the R^2 value, while Figure 5.3 shows the relationships graphically. It is apparent that the final equations are very similar to the initial equations based on simulated data (Figure 5.2) for regions 1 to 3, but that there are quite large differences for regions 4 and 5. A possible explanation is that there are less streamflow gauges used for these two regions, that the initial equations are inappropriate or that there are problems with some of the naturalised flows in these regions. It is also possible that some of the quaternary catchments that have been included in these regions based on simulated flows should really be in other regions. The scatter of the points that made up the last two regions was quite large and it would have been possible to include an additional region or two. However, this would have meant additional regions based on very few data points which would not have been desirable and also it was the intention of the study to keep the number of regions to a minimum. Another pertinent observation is that some of the region 5 catchments are in Lesotho where rainfall is very difficult to estimate. In general, the estimated values of P and PE used in this study are also subject to errors. With P, it is possible that, as is usually the case, the mountainous areas would be poorly gauged and the estimates are not good. The transition from using simulated to naturalised observed data would result in a shift of the points in the

scatter plot. It is thus highly probable that some of the problems could be related to errors in the estimation of these values. The effect may not show up when using simulated data as the simulations are driven by the same P and PE data. However, errors in P and PE estimates could be revealed when using naturalised observed data. The final regions of the runoff ratio constraint illustrated in Figure 5.4 are generally consistent with expectations of the functional behaviour of catchments in the country based on rainfall and evapotranspiration.

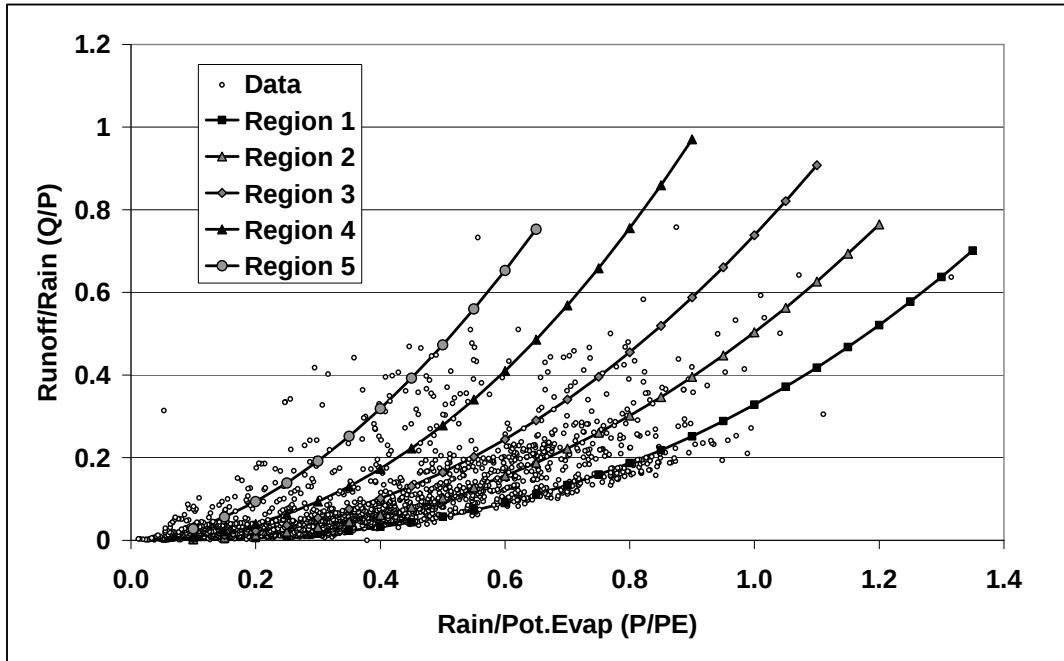


Figure 5.2 Regional Budyko type curves based on log-log relationships using simulated flow data (see Table 5.1 for coefficients of the regression equations).

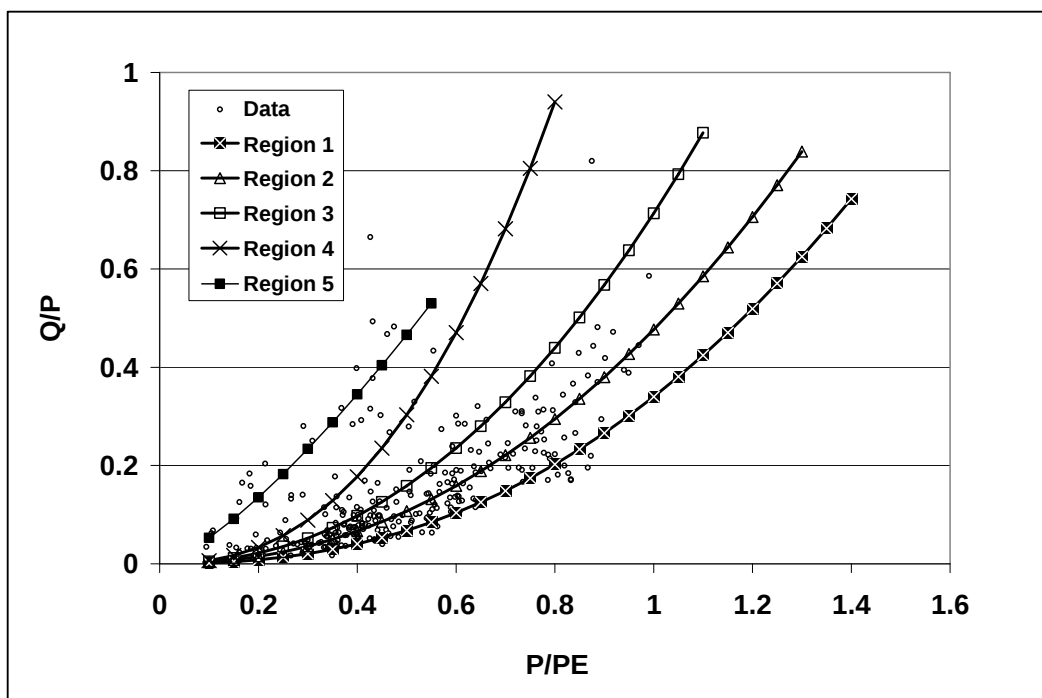


Figure 5.3 Regional Budyko type relationships based on naturalised observed flow data (see Table 5.1 for coefficients of the regression equations).

Table 5.1 Coefficients of the regional Budyko type relationships shown in Figure 5.2 and Figure 5.3

	Regions				
	1	2	3	4	5
Based on simulated data					
No. of basins	397	702	317	202	325
Area (km ²) range	59 – 8647	43 - 18108	72 - 10274	72 - 3913	89 - 8037
Slope (A)	2.527	2.293	2.168	2.126	1.770
Intercept (B)	-1.113	-0.687	-0.304	0.194	0.478
R ²	0.927	0.968	0.984	0.990	0.866
Based on naturalised observed flow data					
No. of gauges	40	135	45	23	27
Area (km ²) range	86 - 1887	81- 1668	106-1691	84- 873	101-1889
Slope (A)	2.322	2.154	2.171	2.406	1.351
Intercept (B)	-1.079	-0.741	-0.338	0.475	0.173
R ²	0.932	0.905	0.890	0.917	0.820

Note: Equations are of the form $\ln(Q/P) = A * \ln(P/PE) + B$

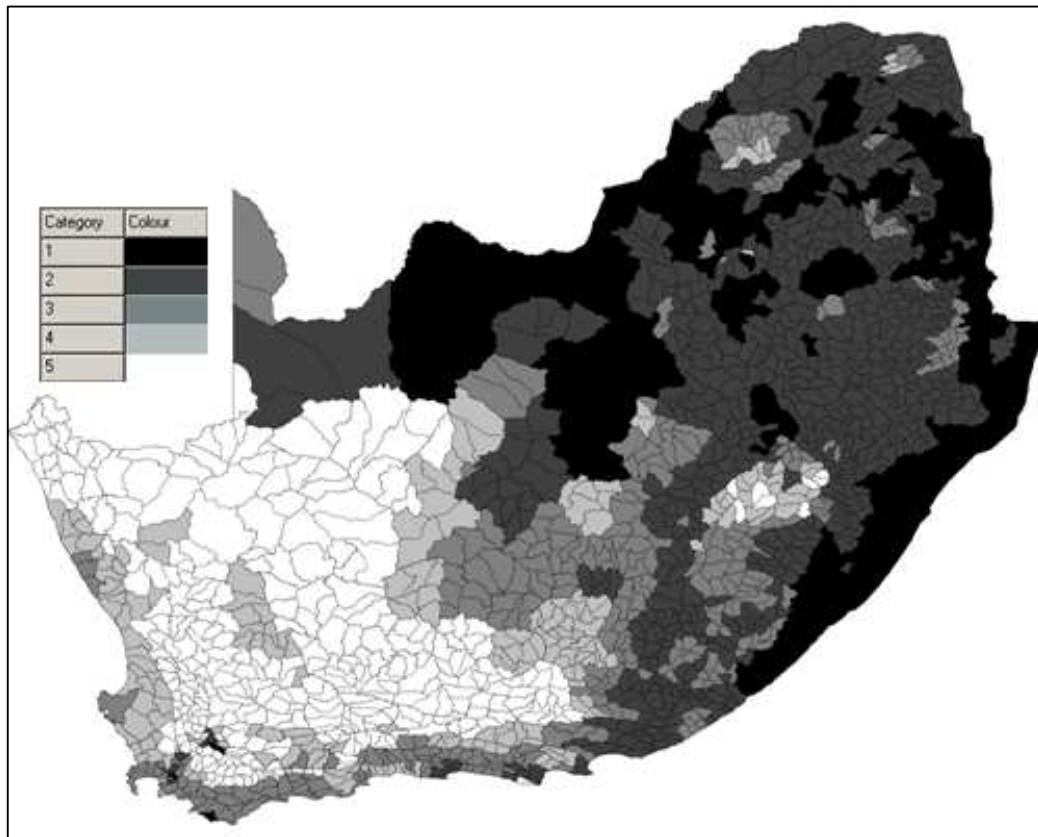


Figure 5.4 Regions based on Budyko type relationships between P/PE and Q/P

5.2.2 Slope of the annual flow duration curve (FDC) for monthly stream flow volumes

The gradient of the flow duration curve (FDC) is a measure of the variability of flows. In a region such as South Africa with very diverse flow regime characteristics, it can be a very useful indicator of hydrological response characteristics. The slope of FDCs is also important in determining potential levels of sustainable abstraction, the need for artificial storage and is relevant to determining environmental flow requirements (Hughes and Hannart, 2003). FDC slope is therefore highly relevant to water resources management.

Development of the constraint relationship

As with the Budyko relationships the starting point for the analysis was to use the simulated flow time series for all 1946 quaternary catchments to try and identify regional relationships. For largely perennial river systems the FDC slope values were calculated as;

$$\text{FDC Slope} = (\ln Q_{90} - \ln Q_{10})/80 \dots\dots\dots 5.1$$

where Q_{10} and Q_{90} are the 10th and the 90th percentiles of the cumulative frequency distribution of flows. For those sub-basins with periods of zero flow, the Q_{90} value was replaced with the first non-zero FDC percentage point value and the difference in flows divided by the appropriate % difference.

Various readily available predictor variables (or combinations thereof) expected to influence FDC shapes were used to try and find suitable estimation equations, either for the whole country or for different regions. It was found to be very difficult to find suitable variables and there were no obvious regional patterns in the data. It has therefore not been easy to regionalize this constraint and it is currently being used on a national scale, while further analyses are still being done to improve the development of a constraint relationship. Figure 5.5 illustrates an interim solution. The estimation equation is based on an index that combines a measure of aridity (P/PE) and a measure of sub-basin slope (relative relief). The equation used is given by;

$$\ln(\text{FDC slope}) = 4.0 - 0.6 * \text{Index value} \dots\dots\dots 5.2$$

where

$$\text{Index value} = \ln(100 * P/PE) + 0.063 * \ln(\text{relief}) \dots\dots\dots 5.3$$

and relief is relative relief estimated from the highest and lowest points in a quaternary catchment using the 90m gridded digital elevation data (<http://csi.cgiar.org>). The R^2 value of the relationship is 0.63 which implies quite wide prediction limits (Figure 5.5). The scaling factor of 0.063 for $\ln(\text{relief})$ was determined by trial and error to achieve the highest possible value of R^2 . The analysis excluded a number of sub-basins in the country that are strongly influenced by dolomitic geology and a region in the north-east of South Africa that appears to be anomalous based on the simulated flow data. The latter group gives values of slope that are difficult to understand based on experience and it was deemed prudent to exclude them to avoid unnecessary and unexplainable noise. Some of the scatter in the relationship as well as the existence of anomalies could be artefacts associated with the use of simulated data.

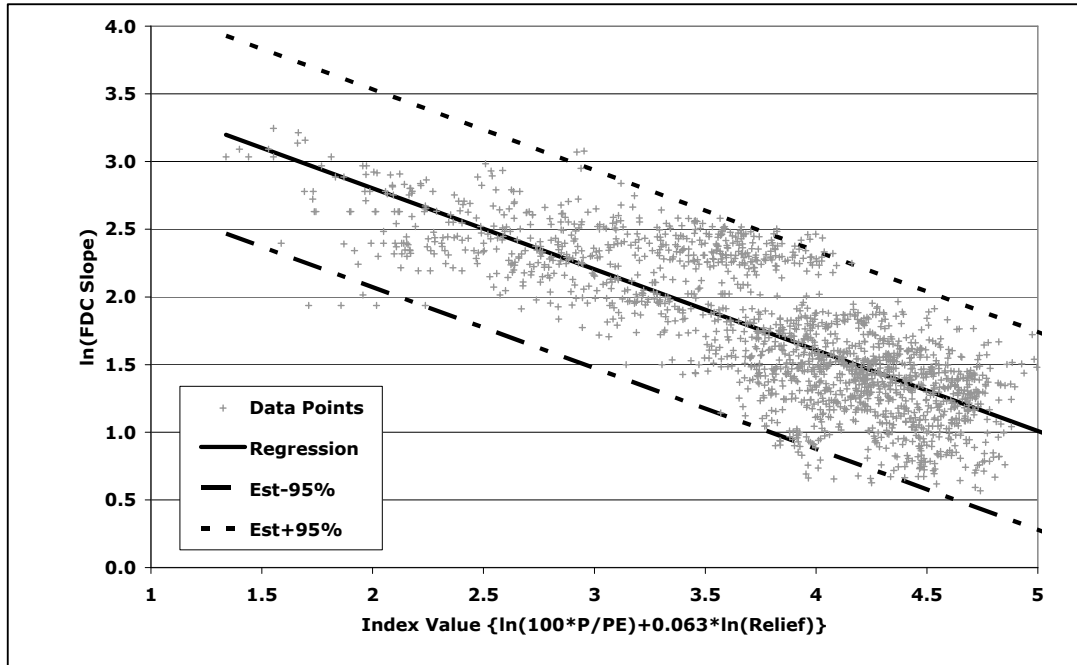


Figure 5.5 Relationships between an index of aridity (P/PE) and sub-basin slope (Relief) and the slope of flow duration curves based on simulated WR90 data (the dashed lines are 90% prediction limits around the regression equation).

The regression analysis was repeated with 230 naturalised observed flow records (taken from WR90, Midgley et al., 1994) and the appropriate format of the index value was found to be closely similar to the one used for the quaternary catchment data (i.e. a scaling factor of between 0.06 and 0.08 for the log value of relative relief). The range of index values is substantially less for the observed data (reaching a minimum index value of only 2.5), the R^2 value is much lower (0.275) but the regression equation is very similar ($\ln(\text{FDC slope}) = 3.64 - 0.53 * \text{Index value}$). The inclusion of relative relief in the analysis of the observed data does not add very much to the precision of the relationship and further work is required to assess other predictor variables that might influence the variability in slope of FDCs. During the analysis of the naturalised observed data no obvious anomalies were apparent which provides some justification for excluding the two groups of catchments (dolomitic areas and some in the North East region) when using simulated data. The problems encountered are possibly artefacts of modelling. This constraint is therefore used here in this form (i.e. on a national scale and not regionalised) as part of this study is to assess the merits of the constraint approach to model application especially in ungauged basins.

5.2.3 Groundwater recharge

During the revision of the initial parameter estimation procedures (Kapangaziwiri and Hughes, 2008), an attempt was made to estimate the main groundwater recharge parameters (GW and GPOW) using estimates of the mean annual recharge (from the GRAII database) and an indication of average soil moisture status based on some of the other parameter estimates. While an estimation approach has been adopted (see Chapter 4, section 4.2.6), initial tests indicated that it can produce dubious and unreliable results and therefore cannot be used with a great deal of confidence. In practice there are too many variables and non-linearities involved in the monthly simulation of recharge within the model to be able to reverse-engineer the model output (i.e. estimate the input parameters required to achieve a defined result in terms of an assumed mean annual recharge). The alternative of using both surface and sub-surface physical catchment properties has yet to be attempted and the results of such an extensive (and more complex) approach cannot be guaranteed to be better than the current approach. Besides, the information on the expected predictor variables is unlikely to be easily available and accessible within the region (Kapangaziwiri, 2008).

Given the relatively low degree of confidence in the recharge parameter estimates it was considered necessary to constrain the ensembles using the GRAII estimates of recharge. It is prudent at this point to highlight the fact that this groundwater constraint is meant to condition one of the internal state variables (related to the representation of the recharge process) of the model and not the final runoff time series that is generated. One of the multiple outputs of the model is a time series of monthly recharge. However, as Figure 5.6 indicates, this is also a highly uncertain process, particularly in those areas where recharge is expected to be high. Figure 5.6 illustrates the ranges of the three different recharge estimates given in the GRAII for all 1946 quaternary catchments. In many cases this range can be in excess of 50mm which would translate into a very wide range of expected groundwater contributions to stream flow. It is worth noting that the largest range is between the middle estimates and the higher estimates, particularly at high recharge rates.

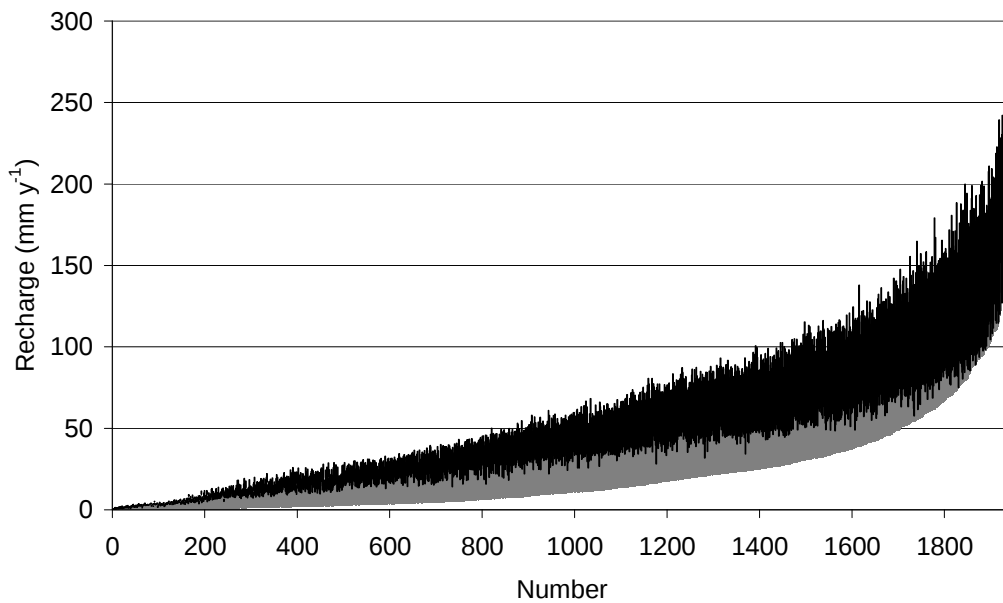


Figure 5.6 Range of mean annual recharge estimates (mm y^{-1}) extracted from the GRAII database for all 1946 quaternary catchments (the results are ranked using the lowest estimate). The grey shaded area represents the difference between the lowest and middle recharge estimates, while the black area represents the difference between the middle and highest recharge estimates.

5.3 Other potential constraints

A number of other potential constraints based on flow characteristics can be investigated and developed in the same manner as described in the preceding sections. These constraints were not used in this study and are intended to be explored in further developments of this work. One of the things that is important to note is that some constraints are model dependent with some more suited to models applied at smaller temporal and spatial scales. It is also important to take cognisance of the quantity and quality of available data on the many different requisite predictor variables (Kennard et al., 2009) for the development of the relationships. Then, there is the need to investigate whether these constraints can be regionalised and whether uncertainty could be added to them so that they can be used to effectively constrain regional model application. Possible constraints include:

- ❖ **Seasonality and year-to-year variability of stream flow:** Stream flow seasonality varies quite substantially in a country like South Africa and indeed in the southern African region and can potentially be used as a

constraint. This variation is a direct result of the timing of peak rainfall and evapotranspiration. Lags between peaks of rainfall and stream flow are naturally expected to vary from shorter delays in the steeper topography of mountainous regions to longer delays in the lower lying, gently sloping areas. Stream flow is most variable from year to year in the arid and semi-arid areas, while wetter regions have less variable regimes. Such an understanding should assist in conditioning model application across different climatic conditions. Capturing such variability into an index which could be regionalised would result in an additional flow metric to assess predictions in ungauged basins. Related to seasonality of flows is the variability of either monthly or annual flows which could also be explored.

❖ ***Number of months of zero flow (or percentage time of zero flows):***

Also used to describe the flow regime of a given basin is the number of months of zero flow or the percentage time of zero flows. This defines the permanency of flow, with drier areas having a larger proportion of zero flows than wetter regions. In some cases where higher flows need to be investigated, regionalisation can be done on the basis of an index based on an average or total duration of pulses above a selected threshold flow or flood/drought frequency (Poff et al., 1997).

❖ ***Coefficient of variation of monthly or annual flows:*** This is also used to characterise variability of monthly or annual flows and depends to a large extent on the hydro-climatic conditions of a basin.

❖ ***Recession coefficients and time-to-peak of the daily hydrograph:*** this is an important criterion for daily or shorter time scale models. Different basins have varied response characteristics to rainfall inputs with shape, area, soil hydraulic properties and slope of a basin being important predictor variables. Such constraints can help determine the flashiness of basins (DeMaria et al., 2007).

5.4 Summary

The objective of finding suitable constraints is to provide a basis for checking which of the many different parameter sets used to generate the ensembles produce behavioural results and therefore reducing the uncertainty in model simulations. However, as pointed out earlier, it should be acknowledged that all of the constraint relationships are also subject to uncertainty. This uncertainty is related to:

- ❖ The accuracy of the data used to calculate the dependent variables of the constraint relationships (i.e. indices of hydrological behaviour). In the case of South Africa this involves the use of stream flow data that contain measurement errors and a wide variety of effects of upstream water resources developments and land use impacts. The data being used in this study are therefore the corrected and naturalised data. The impact of this naturalisation process has not been assessed. Questions can still be raised as to this impact. Could this have been done differently? It is possible that that may lead to different regional equations/relationships or some basins may transfer to different regions. Unfortunately, the assumptions that were used for naturalisation and correction are not documented and therefore cannot be checked. It must be acknowledged that the information available during the WR90 (Midgley et al., 1994) study upon which to base a naturalisation would have been less than ideal.
- ❖ The data used as independent variables in the constraint relationships are subject to either error or generalisation (smoothing) at the catchment scale.
- ❖ The choice of independent variables for use in the constraint estimation equations is limited to information that is readily accessible and may not necessarily be the most appropriate for a specific constraint.

One of the fundamental questions that are very difficult to answer is which of the estimation approaches used in this study is subject to the most unknown uncertainty. Is it within the methods used to develop the constraint relationships, or is it in the methods used to estimate the parameter values? The whole basis of the framework presented in Chapter 3 is that the constraint relationships can be used to determine which of the different model parameter sets are used to generate the ensembles behavioural. The assumption is therefore that the constraint relationships are determined with less uncertainty than the parameter sets. Whether this is a realistic assumption remains to be seen. The initial intuitive indications would be that high confidence can be expressed in some of the constraint relationships (e.g. the volume constraint based on the relatively high R^2 values – see Table 5.1), while others will remain very uncertain unless improved relationships can be developed (e.g. the poor R^2 value for the FDC slope) or unless better data can be used to develop the constraints (e.g. the very wide range of recharge estimates that are currently available). An attempt at

exploring this issue will be further discussed during the presentation of the results.

CHAPTER 6

TOOLS DEVELOPED TO IMPLEMENT THE FRAMEWORK

6.1 Introduction

Having discussed the main tenets and components of a framework of model application in the region (Chapter 3), the next logical task was to look at framework implementation. This chapter, therefore, aims at describing the tools that are used for the implementation of the framework. The implementation tools are the techniques and/or software developed for use within the framework. They are intended to facilitate effective execution of the framework and to increase the probability that users will take objective and consistent actions to generate consistent and hydrologically plausible results. The tools that have been developed include the parameter estimation software, Pitman model modifications to allow Monte Carlo simulations and regional sensitivity analysis software. These tools were all developed in the Delphi programming language and designed to be compatible with existing modelling software used within the Institute for Water Research (IWR) at Rhodes University. While the parameter estimation software is a new development for the Pitman model, the others are adaptations of popular existing methods. The main aim of the framework and the implementation tools is to provide efficient, relevant and practical hydrological modelling solutions that can benefit water resources management and planning.

The Pitman model operates within a database and information management platform known as SPATSIM (Spatial and Time Series Information Modelling, Hughes and Forsyth, 2006). SPATSIM is an integrated hydrology and water resource information management and modelling system which makes use of ESRI Map Objects and the Delphi programming language to create a data management environment with a spatial information front end and a relational database structure to provide access to a wide range of different types of hydrological and water resource information. The package includes many utilities for importing data of all types, viewing, graphically displaying and editing data, sharing data with other users and further processing data to create new information. It also provides access to a wide range of linked models and data analysis procedures that are typically used in water resource assessments (rainfall-runoff models, design floods, reservoir water balance models) and

ecological water requirement assessments (Hughes and Forsyth, 2006). All data are stored in a database and all the software tools currently operating on this platform are capable of reading from and writing to the database. The new software tools (parameter estimation and regional sensitivity analysis) developed to support the implementing of the framework are currently stand-alone applications, which can either generate outputs that can be easily imported into SPATSIM, or they use data generated by SPATSIM. The outputs of the parameter estimation program (i.e. the parameters and the distribution characteristics) are used as the input into the Pitman model to simulate output ensembles. These ensembles are direct inputs into the regional sensitivity analysis program. Once the design of these tools has been finalized, they will be fully incorporated into the SPATSIM system.

6.2 Parameter estimation software

The process of parameter estimation incorporating uncertainty was fully described in Chapter 4 and this section is an overview of the software that facilitates the application of the estimation process. The section is essentially provides an explanation of the coding or operationalisation of the detail given in Chapter 4. The parameters are estimated directly from inputs of physical basin attribute data. The uncertain model inputs (in this case, parameters) are defined by distributions. These distributions are based on the assumed uncertainty in the basin physical and hydro-climatic predictors used to quantify the parameters. The software developed for this makes use of the principle of Monte Carlo sampling from the assumed distributions of the predictor variables to generate a sample of the population of possible values of the estimated variable. From this sample, a posterior distribution function of the estimated variable is defined. In the software this estimated variable could be a basin scale equivalent of the basin physical property or an estimation of a physical derivative necessary for basin scale estimations or a parameter. The software that performs these tasks therefore has three basic components:

The primary inputs: these are the raw physical basin data measured at smaller than the sub-basin scale which is the modelling scale. These are mainly made up of soil texture and type classes, soil depth, terrain unit slopes and geology. Also making up part of the primary inputs are basin hydro-climatic data, for example monthly rainfall, number of rain days, annual recharge, etc.

Calculation of secondary variables: these are sub-basin scale estimates of the physical basin attributes data and other derivatives of these data, for example porosity, permeability, etc. They are intermediate estimates for the parameter estimation procedures. Translation equations are applied to the relevant primary inputs to derive these variables (Section 4.2).

Determination of the model parameters: based on equations developed in Chapter 4 and Kapangaziwiri (2008), the primary basin inputs and/or the secondary basin variables are used to calculate sub-basin scale values of parameters.

The calculations used for the estimation of the frequency distribution properties of secondary basin variables and parameters make use of Monte Carlo sampling to generate a sample of predetermined size from which the distribution statistics (mean, standard deviation and skewness) are estimated. The distribution properties of the necessary secondary inputs are calculated first through sampling from the distributions of the primary inputs. These are then used to calculate parameters. The results of these calculations are the estimates of parameters of the model, some with uncertainty while others are estimated without uncertainty. However, some of the parameters that are not part of the estimation process have their default values written out at the same time. This is to ensure that the full complement of parameters is written out and can easily be imported directly into the model without having to first organize the output file. For those parameters estimated with uncertainty, the mean value of the parameter, its standard deviation, skewness and a distribution type are specified. The final part of the output text file is compatible with the parameter input data to the Pitman model (see Section 6.3 and Table 6.1). The results are output to a text file which can be modified and can be imported back into the program so that changes to an existing set of data can be made (i.e. save existing data).

6.3 Pitman model modifications

The aim of this section is to describe the modifications made to the SPATSIM version of the ground water version of the Pitman model (Hughes and Parsons, 2005) to enable it to manage the input probability distributions of the uncertain parameters and generate ensembles of simulation outputs using a Monte Carlo sampling technique. This process is represented in Figure 6.1.

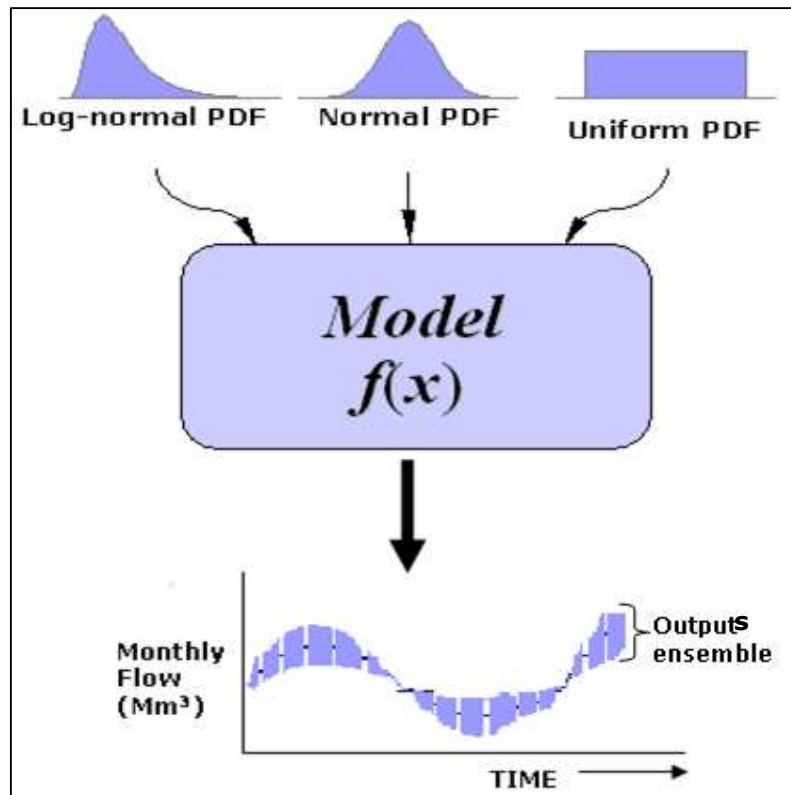


Figure 6.1 Diagrammatic representation of the uncertainty version of the Pitman model.

Each parameter can be input with uncertainty represented by one of three distribution types (Normal, log-Normal or Uniform) i.e. uncertainty is expressed through a range of possible values instead of a single value. Table 6.1 lists the contents of the uncertain parameter inputs to the model and is identical in format to the final part of the text file output from the parameter estimation program. The six data columns for each model parameter represent:

- ❖ The mean value of the parameter which is used to represent the mean of a Normal distribution or is the logarithmic value of the mean of a log-Normal distribution. It is assumed to represent the 'best guess' of the parameter value.
- ❖ The standard deviation of the parameter which is used directly if a Normal distribution is specified. If a log-Normal distribution is to be used, the natural log of this value represents the standard deviation. If this value is 0 the parameter is assumed to be estimated with no uncertainty (thus calculations will use only the mean value) regardless of any other settings.

- ❖ The skewness of the distribution which is included for information purposes only and is not used in the model.
- ❖ The distribution type, where 0 represents no uncertainty, 1 a Normal distribution, 2 a log-Normal distribution and 3 a Uniform distribution.
- ❖ Minimum and maximum values. If either a Normal or a log-Normal distribution type is specified, these represent the limits of the sampling process and sample values for parameters generated outside these limits are rejected in the Monte Carlo process. Currently the values are set arbitrarily. However, it is possible to narrow or widen the ranges if detailed information is available. If a Uniform distribution is specified, these values represent the limits of the distribution and all values between them are considered equally probable.

For each run of the model, a parameter set is generated through Monte Carlo sampling from within the distributions of the input parameters. The number of model runs (and therefore the number of parameter sets and output ensembles) is set to 5000 by default but can be specified by the user (Figure 6.2). If a Uniform distribution has been specified, a uniform random deviate (RND) between 0 and 1 is generated (using the random sample generation procedure given in Press et al., 1988) which is then scaled using the minimum (P_{MIN}) and maximum (P_{MAX}) parameter values to give the value used in the model run (P):

$$P = RND * (P_{MAX} - P_{MIN}) + P_{MIN} \dots\dots\dots 6.1$$

If a Normal or log-Normal distributions has been specified a normally distributed deviate (NRND), with a mean of 0 and a standard deviation of 1, is generated (using the random sample generation procedure given in Press et al., 1988) which is scaled using the mean (P_{MEAN}) and standard deviation (P_{SD}) values for the parameter. For a Normal distribution type:

$$P = P_{MEAN} + NRND * P_{SD} \dots\dots\dots 6.2$$

And for a log-Normal distribution type:

$$P = e^{(\ln(P_{MEAN}) + NRND * \ln(P_{SD}))} \dots\dots\dots 6.3$$

and for both cases, $P \geq P_{MIN}$ and $P \leq P_{MAX}$.

It is important to note that the samples for each parameter are independent of the other parameters within a sub-basin and that each parameter is sampled independently across all sub-basins within the spatial distribution system. This is an attempt to preserve the physical integrity of the model. It is assumed that without this independence the individual impacts of the sub-basins may be understated or overlooked. From Table 6.1 it can be seen that uncertainty can be associated with all of the input parameters of the models, while only the natural hydrology parameters are included in the parameter estimation program. Therefore, it is possible for users to include the effects of such influences as farm dams (Hughes and Mantel, 2010) or irrigation abstraction developments in the uncertainty analysis. However, estimating the statistics on the uncertainties for these parameters would have to rely on the methods that are not included in the framework at this stage.

The parameter estimation process discussed in Section 6.2 assumes that the parameter distribution will be either Normal or log-Normal, based on the assumption and interpretations of the physical basin property data that were discussed in Chapter 4. This implies that some parameter values are more probable than others. If this implication cannot be supported by the available information then it will almost always be more appropriate to use a uniform distribution with minimum and maximum values set to realistic limits. This issue is mostly relevant to any of the parameters that have not been included as part of the parameter estimation process, or where the data used in this process (AGIS, 2007) are not available.

Table 6.1 An example of the input parameter table for use with the uncertainty version of the Pitman model.

Parameter	Mean Value	SDev Value	Skewness	Dist. Type	Minimum	Maximum
Rain Distribution Factor	1.28	0	0	0	0	0
Proportion of impervious	0	0	0	0	0	0
PI1 Summer	1.955	0.282	0.254	1	0	5
PI1 Winter	1.954	0.284	0.266	1	0	5
PI2 Summer	3.985	0.021	-0.005	1	0	5
PI2 Winter	3.985	0.022	0.001	1	0	5
% Area of Veg2 (AFOR)	20	0	0	0	0	0
Veg2/veg1 Pot. Evap.	1.4	0	0	0	0	0
Power of veg (not used)	0	0	0	0	0	0
Annual Pot. Evaporation	1400	0	0	0	0	0
Summer ZMIN	61	11.503	-2.798	1	0	200
Winter ZMIN	61	11.503	-2.798	1	0	200
ZMEAN	233.127	0	0	0	0	0
ZMAX	1027.4	35.122	-0.114	1	0	5000
ST (mm)	174.792	28.259	0.026	1	10	5000
SL (Min Recharge S)	0	0	0	0	0	0
POW	2	1.01	9.97	2	1	10
FT (mm)	4.963	1.614	0.175	1	0	1000
GW	14.282	2.833	1.246	1	0	1000
R (Evap/storage relation)	0.5	0	0	0	0	0
TL (Surface Q delay)	0.25	0	0	0	0	0
CL (Channel Routing)	0	0	0	0	0	0
Irrigation Area	0	0	0	0	0	0
Return flow fraction	0	0	0	0	0	0
Effective Rainfall	0	0	0	0	0	0
Non Irrig Direct Demand	0	0	0	0	0	0
Max. Dam storage	0	0	0	0	0	0
% Area above dams	0	0	0	0	0	0
A in Area = $A \cdot vol^B$	0	0	0	0	0	0
B in Area = $A \cdot vol^B$	0	0	0	0	0	0
Irrig. Area from Dams	0	0	0	0	0	0
Channel Loss TLGMax	0	0	0	0	0	0
GPOW	3	0	0	0	0	0
Drainage Density	0.4	0	0	0	0	0
Transmissivity	8	1.6	0	1	1	500
Storativity	0.002	0	0	1	0.001	0.8
Regional GW slope	0.01	0	0	0	0	0
Rest water level	25	0	0	0	0	0
Riparian Strip Factor	0.2	0	0	0	0	0
GW Abstraction (Upper)	0	0	0	0	0	0
GW Abstraction (Lower)	0	0	0	0	0	0

Note: • Dist Type refers to the distribution type used in the uncertainty analysis. 1 and 2 indicate where the normal and the log-normal probability distributions respectively were used. 0 indicates where no uncertainty was considered.

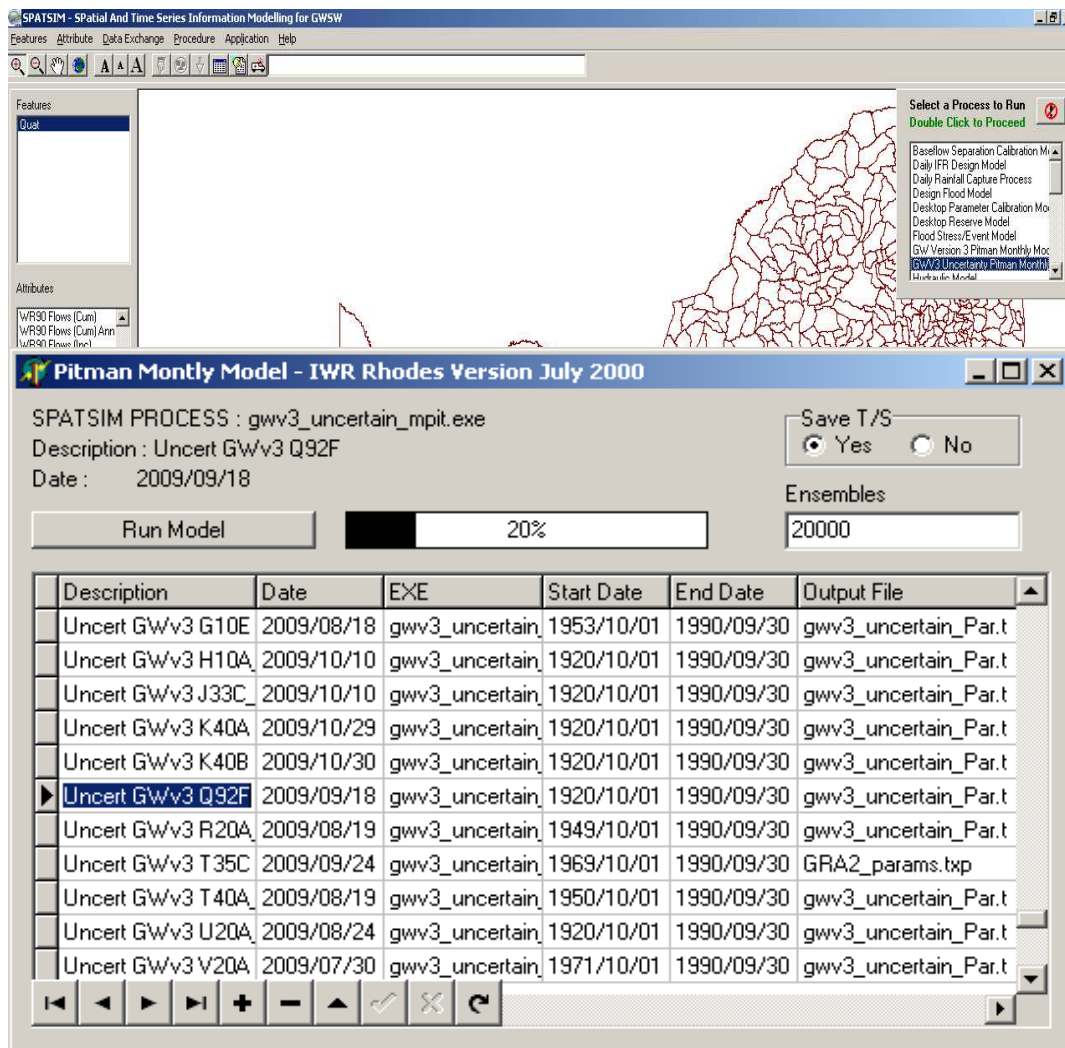


Figure 6.2 Screenshots of the uncertainty version of the Pitman model showing a model run for basin Q92F set to generate 20 000 output ensembles. The upper part of the diagram shows the SPATSIM step to choose a process (or model) to initiate.

Model Outputs

The model produces ensembles of simulated flows (Figure 6.1) which are saved as time series in the SPATSIM database. Additional outputs are saved to two separate text files, with .un1 and .un2 extensions. The full name of the files is given in the form pitmV3_ (basin ID).un1; for example the .un1 and .un2 files for basin Q92F will be written as pitmV3_Q92F.un1 and pitmV3_Q92F.un2 respectively. The .un1 file contains the list of sampled parameter values, the simulated mean monthly runoff volume ($\text{m}^3 \times 10^6$), the simulated mean monthly recharge (mm), the slope of the flow duration curve (FDC) and the 10th, 50th and

90th percentiles (as volumes in m³ * 10⁶) on the annual FDC for each of the outputs. The first is used for the volume (runoff ratio) constraint, the second for the recharge and the third is the slope of the FDC constraint. If observed data are available and have been included as part of the model setup, five objective functions are also written out for each of the ensembles. These are the Nash coefficient of efficiency (CE, Nash and Sutcliffe, 1970) for untransformed values, natural logarithm transformed and inverse values and the percentage difference of mean monthly flows for untransformed and natural logarithm transformed values. Zero flows are ignored when using the natural logarithmic transformation. CE is one of the most widely used measures of goodness-of-fit in hydrological modelling. It is a dimensionless index of correspondence between the simulated and observed time series. It is written mathematically as:

$$CE = 1 - \frac{\sum (Q_{obs} - Q_{sim})^2}{\sum (Q_{obs} - \mu_{obs})^2} \dots\dots\dots 6.4$$

where Q_{obs} is the observed time series, Q_{sim} the simulated time series and μ_{obs} is the mean of the observed series. CE can assume any values between $-\infty$ and 1 with the latter indicating a perfect fit between the observed and the simulated flows. When CE takes the value of zero, the simulated flow is no better estimator than the mean of the observed flows and a negative value indicates that the simulated flow is a worse estimator than the mean observed flow. CE has been observed to give relatively high values even for some visually poor simulations. It is also difficult to get high CE values in basins or periods where the variation of streamflow is low. The value of CE is sensitive to systematic errors.

The percentage error of the mean monthly runoff (MMR) is a measure the percentage deviation in the mean monthly flow of the simulated from the observed. A perfect correspondence between the hydrographs results in a value of zero with poor simulations being shown by an increasing divergence from zero. Low, near zero values of this objective function would be an indication of low bias, high positive values would indicate an under-estimation of the historical observed flows, and high negative values would indicate an over-estimation. If the absolute value is considered, then a high value would indicate a systematic error (often referred to as bias). This objective function can be expressed mathematically as:

$$\%Mean = 100 * (MMR_{obs} - MMR_{sim}) / MMR_{obs} \dots\dots\dots 6.5$$

where MMR_{obs} and MMR_{sim} refer to the MMR of the observed and simulated time series respectively.

The .un2 text file (written as pitmV3_(basin ID).un2) contains four columns of monthly flows for each month of the simulation period. The first three columns are the 5th, 50th (i.e. the mean) and 95th percentiles of the monthly flows of the output ensembles. For any month of the modelling period, all the model outputs (number depends on the number model runs specified, 5000 being the default) for that month are ranked and the percentiles are calculated. It should be noted that these do not represent actual simulated time series, but are the bounds within which 90% of the output ensembles would fall. This is necessary in order to draw the envelope around the ensemble outputs and determine the full range of output uncertainty. A narrow range would reflect less uncertainty and may indicate higher chances of the parameters being identifiable. The final time series (fourth column) is a copy of the 'observed' data passed to the model from SPATSIM for reference purposes (if included in the model setup). These 'observed' values could be real historical observed flows from a gauging station or could be some other reference time series used for comparison with the simulated outputs ensemble (e.g. in South Africa, the WR90 or WR2005 simulated flows, used for water resources estimations and planning as the national 'conventional wisdom' can be used in the absence of observations). The contents of .un2 can be presented together with the ensembles as in Figure 6.3.

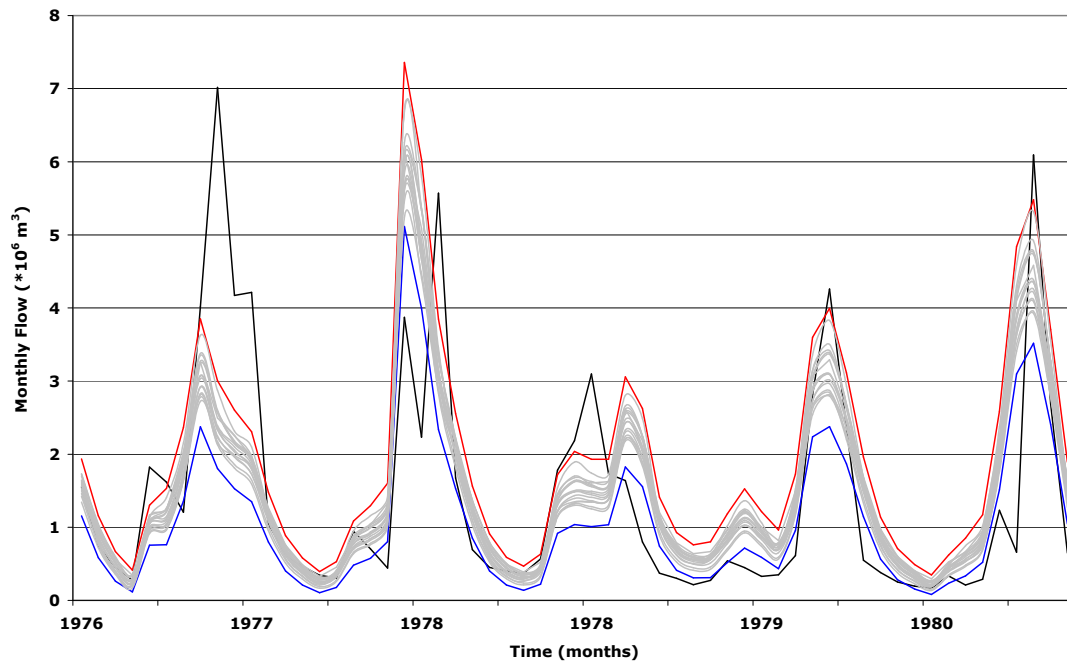


Figure 6.3 An illustration of the presentation of the contents of the output file .un2. The black, red and blue graphs represent the observed flow, 95th percentile and 5th percentile respectively. The grey graphs are samples of model output for a sub-basin (V60A) of the Sundays River in the Tugela River system V60A.

The contents of the .un1 text files (i.e. output ensembles) can be analysed in either the regional sensitivity analysis software (Section 6.3) or in excel spreadsheets. Using the later it is possible to perform an overall uncertainty assessment for the Pitman model by comparing the uncertainty generated through the parameter estimation process with that resulting from the various constraints (see Chapter 6). To define the limits of acceptability of the outputs based on the constraints, the $\pm 95\%$ prediction interval about the regional (where applicable) regression equations are determined. The prediction limits are derived from the characteristics of a standard Normal distribution (with mean 0 and standard deviation 1) where the 95% of the distribution falls within ± 2.2 standard deviations about the mean. When considering the constraints, a standard deviation (σ) for any given region is calculated and then used to determine the boundaries of the prediction interval about the graph of the regression

relationship. For instance, for the runoff ratio constraint, the general equation is given by;

$$\ln(Q/P) = A * \ln(P/PE) + B \dots\dots\dots 6.6$$

where A is the slope and B is the intercept of the regression relationship. The limits of the prediction interval (5th and the 95th, representing respectively the lower and upper limits) would be given by;

$$e^{[A * \ln(P/PE) + B \pm 2.2\sigma]} \dots\dots\dots 6.7$$

The members of the output ensembles are then used to calculate the constraint metrics. For each metric, the results are then compared with the regional constraints in a simple plot as illustrated in Figure 6.4.

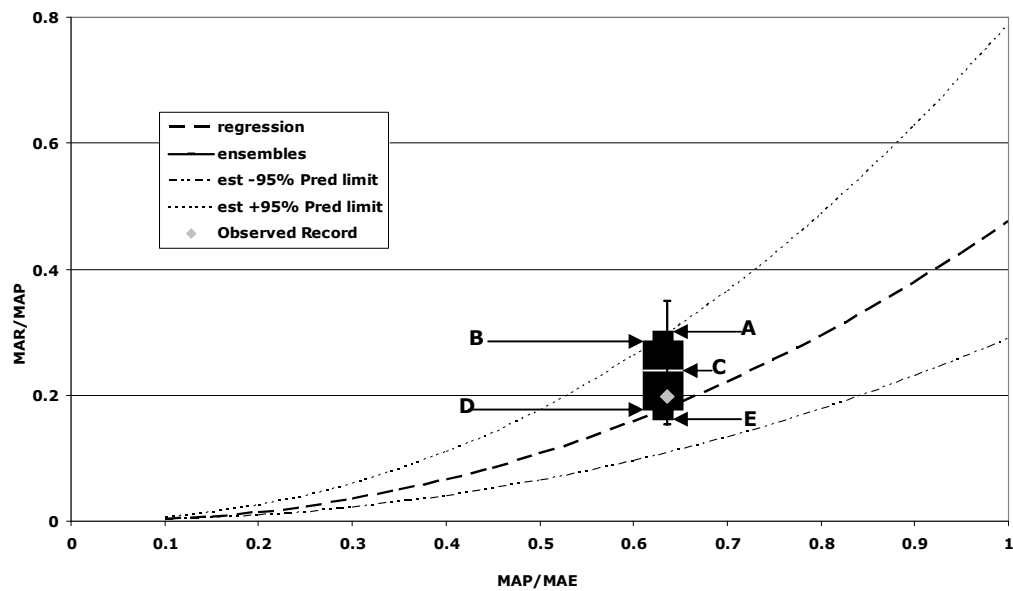


Figure 6.4 An example of the runoff ratio analysis for a sub-basin (V60A) of the Sundays River in the Tugela River system. Also shown are simple statistical properties of the output ensemble, marked A to E respectively representing the 2.5th, 5th, 50th (median), 95th and 97.5th percentiles. The minimum, A to E and maximum runoff ratio values are 0.17, 0.20, 0.21, 0.23, 0.27, 0.28 and 0.35 respectively.

Figure 6.4 shows that the observed constraint metric (Q_{obs}/P) falls within the simulated outputs ensemble and within the regional boundaries of expected

behaviour. The ensembles show a bias toward somewhat higher flows than the regional constraint prediction limits and 0.3% of the outputs lie above the 95th percent prediction limit. In terms of the proposed framework these would be considered non-behavioural. The outputs that fall outside the regional constraint boundaries can be further analysed to try and identify which parameters, or groups of parameters, have resulted in these non-behavioural results. Such analysis could indicate problems with the parameter estimation equations or the way in which the physical basin data have been interpreted. Simple scatter plots of the parameter values against the objective functions (or constraint metrics) can be used to examine the identifiability of individual parameters (Figure 6.5). Based on these plots a parameter would be deemed identifiable if there is a distinct maximum in the scatter plots and the absence of such a distinct maximum indicates the difficulty to find a single optimal value that provides good model performances, hence the parameter is termed poorly identifiable.

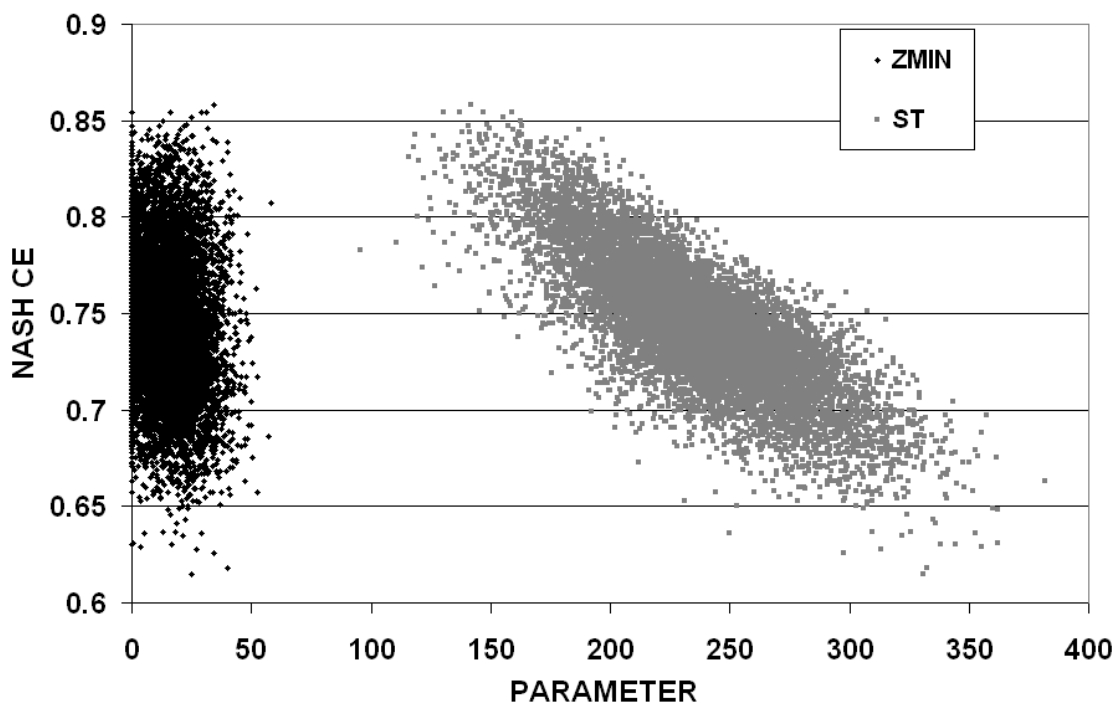


Figure 6.5 An excel plot for the analysis of identifiability of parameters ZMIN and ST for V70D (Little Boesmans river), a sub-basin of the Tugela river basin.

Figure 6.5 therefore suggests that the optimal values are lower than the ST values used in the ensemble generation. There is no clear optimal value for the

parameter ZMIN. It is also possible to use facilities in SPATSIM to display and analyse the model outputs ensemble. This can be achieved using the TSOFT facility. TSOFT is a generalised time series graph display and analysis software package provided with SPATSIM. TSOFT is designed to work with data reference files called 'Profiles Files' and these can contain references to records in a database table (such as a SPATSIM time series attribute table) or to binary files generated by different models and stored in the database (Hughes and Forsyth, 2006). To use this facility, one needs to create this profile (saved as a .prf file) first and then specify the data (time series attributes) that will be contained in this profile. Figure 6.6 shows a TSOFT display of 10 members of the simulation outputs ensemble (size 20 000) for a sub-basin (V60A) of the Sunday River.

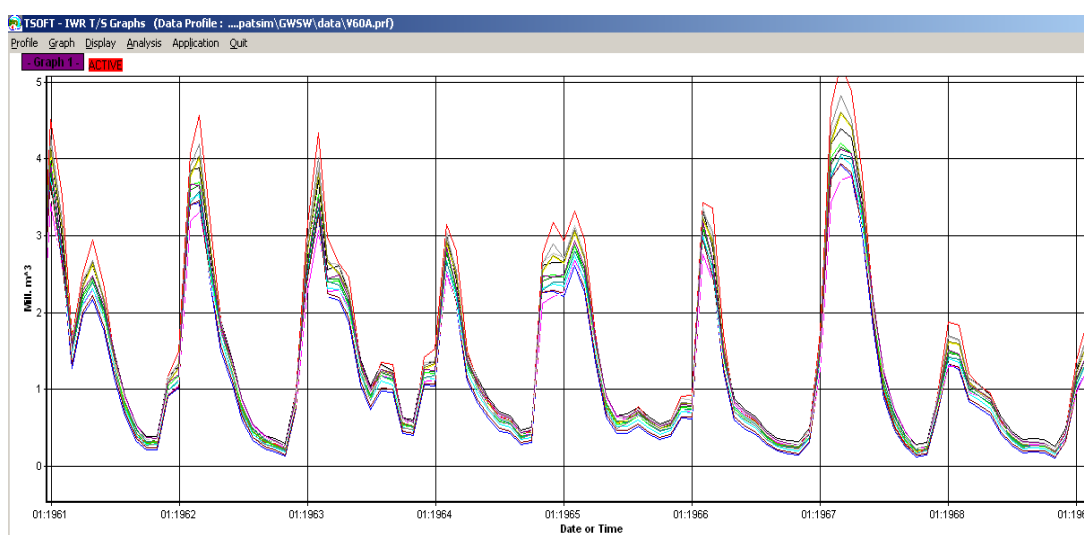


Figure 6.6 A screen shot of the TSOFT display of 10 output ensemble members from the simulations of V60A on the Sundays River, a sub-basin of the Tugela River basin.

6.3 Sensitivity Analysis

The analyses of the model output ensembles through excel spreadsheets only identify the extent of variability in any given basin and, therefore, potential problem basins where the output uncertainty due to the parameter estimation process is higher than the constraints uncertainty. While the constraints can illustrate the extent of this uncertainty and identify those ensemble members that are not consistent with natural phenomena and/or expected hydrological behaviour, they fail to inform the identification of the parameters and/or

parameter combinations that lead to this inconsistency. Indeed, they reveal little about the sensitivity of the model predictions to the individual parameters, except where some strong change in the likelihood measure is observed in some range of a particular parameter (Freer et al., 1996). The model output surface is a product of the combined effects of the parameters and interactions between/among them within any given model structure. It is therefore prudent to assess the impact of individual parameters on the output space. Sensitivity analyses can be used to determine the impact of individual parameters on the constraints, and a software tool has been designed for this purpose based on techniques reported in the literature (Wagener et al., 2001; Freer et al., 1996). General sensitivity analysis aims at determining how the uncertainty in the model output can be apportioned (qualitatively or quantitatively) to different sources of uncertainty in the model inputs (Saltelli et al., 2008). In essence one looks at the effect of varying the inputs of the model on the expected outputs. If the impact is small, the model can be simplified either by replacing the relevant parameters by constants or by eliminating them altogether (Wagener et al., 2001). In the current study only parameter uncertainty is being looked at and the effect being analysed is that of the individual parameters on the model output. While the effects may be masked within broader uncertainty by many other sources including rainfall input and model structure, it is hoped that these will tend to be systematic given that the rainfall input and model structure have been not been varied. The impact of rainfall and model structure will be investigated in future research.

Most contemporary sensitivity analysis techniques are derivatives of the regional sensitivity analysis (RSA) ideas of Hornberger and Spear (1981), Leamer (1990) and/or their refinements by later workers like Freer et al., (1996). Leamer (1990) suggested that sensitivity analysis is where, "a neighborhood of alternative assumptions is selected and the corresponding interval of inferences is identified. Conclusions are judged to be sturdy only if the neighborhood of assumptions is wide enough to be credible and the corresponding interval of inferences is narrow enough to be useful". The basic idea of a sensitivity analysis involves a comparison of the model output ensembles against a chosen assessment criterion which could be an objective function or any given flow metric (e.g. any of the constraints). In principle the RSA method evaluates sets of parameter values in terms of model performance without making assumptions about their frequency distribution characteristics (Demaria et al., 2007) and is based on a Monte Carlo

sampling of the parameter space (Hornberger and Spear, 1981; Freer et al., 1996).

The implementation of the RSA method adapted for this study is related to the way it is used in the Monte Carlo Analysis Toolbox (MCAT, Wagener et al., 2001) and is based on the modifications by Freer et al. (1996) which do not rely on a determination of a threshold to distinguish between behavioural and non-behavioural parameters (Demaria et al., 2007). While the Wagener et al. (2001) method ranks the model output ensemble on the basis of a chosen objective function, the sensitivity analysis tool used in this study can also rank the outputs using the constraint metrics. This approach is more robust as it assesses the impact of the parameters (and any other source of uncertainty that may be considered) where there are no historical records. This represents an alternative approach to RSA that can be applied in ungauged basins. Until now, it has not been easy to do a sensitivity analysis in ungauged basins because either the determining of the performance or behaviour thresholds or the use of objective functions presupposes the existence of reasonably accurate historical records. Such records are not readily available in the region (Kapangaziwiri, 2008).

Firstly, using the .un1 files, the output ensembles are ranked on the basis of the assessment criterion (either an objective function or any flow metric included in the output file) and then sorted into five equal groups. While any number of groups can be used, five are deemed sufficient for the purposes envisaged for the program and for ease of display of the results. The normalised cumulative frequency distribution of the parameters of each group is then plotted with respect to the model performance based on the selected objective function or with respect to the selected metric to assess the impact of individual parameters. If a flow metric is selected that forms part of one of the regional constraints (mean monthly flow or the slope of FDC, see Figure 6.7) an additional two groups can be created. The information entered in D of Figure 6.7 is used together with the constants of the constraint regression equation (currently hard-coded within the program) to calculate the 95% prediction limits. Any of the ensembles falling either above or below these limits are extracted into the 'above behavioural' and 'below behavioural' groups (Figure 6.8) and plotted separately. The remaining ensemble members are equally divided into the 5 main groups discussed above.

Figure 6.7 shows a screen shot of the setup screen for the program that allows the user to select the parameters and the assessment. The top row of Figure 6.7 indicates the .un1 file that has been loaded and the number of ensemble

members within the file. The top left hand side window contains all the parameters of the model, from which a maximum of 9 can be selected for analysis. The limitation of 9 parameters is related to the number of graphs that can be displayed on a standard computer screen without making them too small. After highlighting the parameters for assessment, these are loaded into the bottom left hand side window by double clicking in the window (labelled 'parameters selected'). The assessment criteria are given in the circles A and B, where A is the group of flow metrics and B is the group of objective functions. The chosen assessment criterion is loaded into C. If one chooses to use any of the flow metrics, then D is activated and the user will need to input the data required which includes the region number (from the regionalised constraints), the basin area (km², this would be the cumulative area in the case of multiple contiguous sub-basins), mean annual precipitation (mm), mean annual potential evaporation (mm) and elevation range (m). These are necessary for the determination of the ensemble members that lie inside or outside the constraint boundaries. The 'Go' button is used to perform the analysis after all the necessary selections have been made.

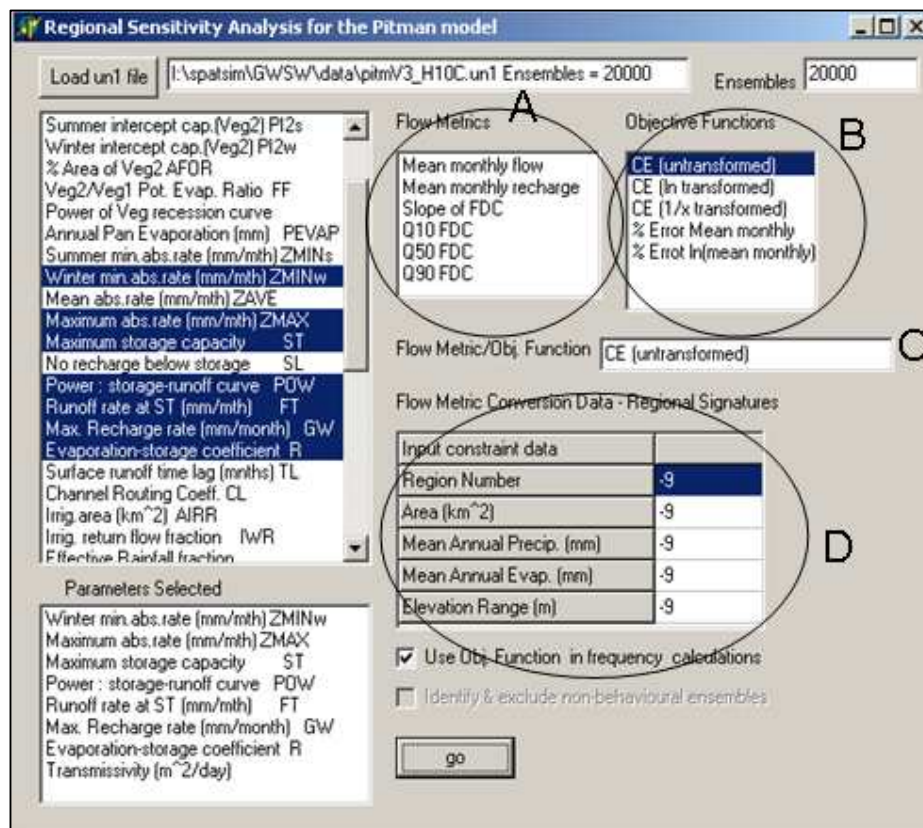


Figure 6.7 Screenshot of the regional sensitivity analysis tool.

Figure 6.8 provides an example of the sensitivity analysis results. The sensitivity of individual parameters is measured by the degree of divergence between the normalised cumulative frequency curves of the five groups. The wider the separation of the curves indicates that the parameter under review is very sensitive based on the assessment criterion selected. Figure 6.8 shows that parameters GW, FT and POW are the most sensitive, while PI and ZMIN are the least sensitive. If an objective function assessment criterion has been selected, the diagrams can be used to indicate the range of parameter values that give the best result. However, problems with equifinality often result in this range being quite large (e.g. 10 – 30 mm/month) for GW in Figure 6.8. Frequency curves that are steep and where the top and lower 20% lines are well separated suggest identifiable parameters, none of which is evident in Figure 6.8.

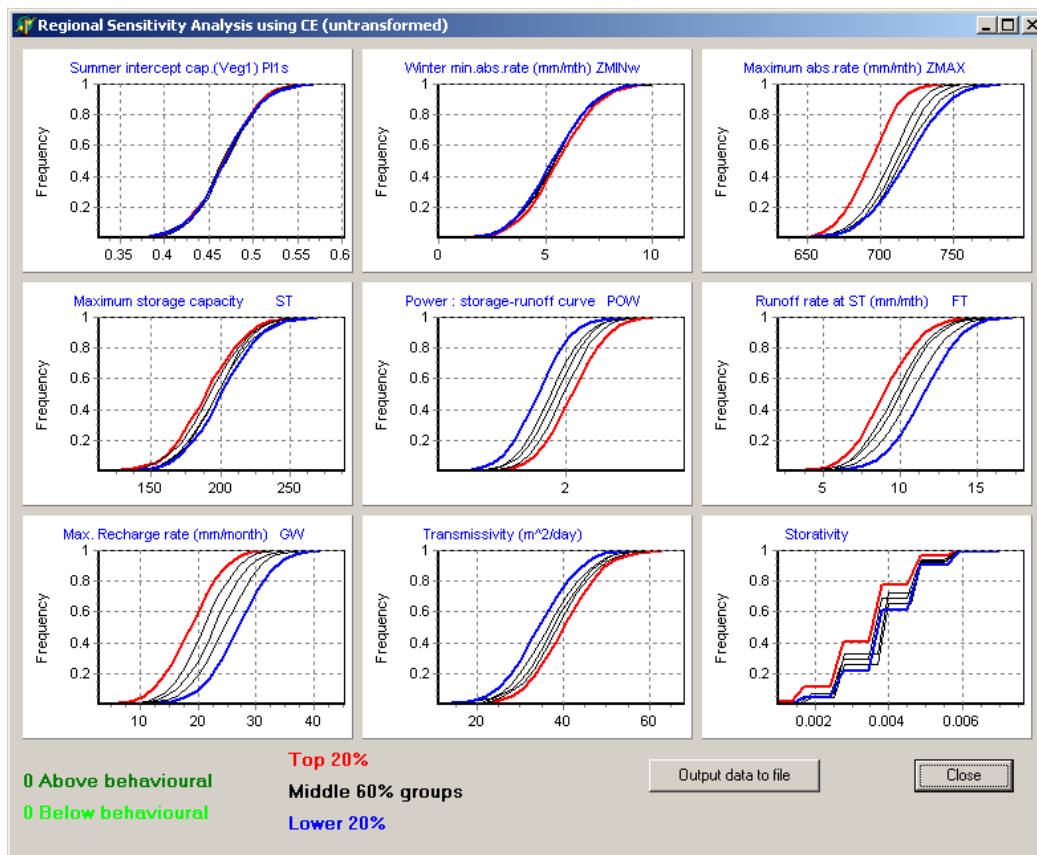


Figure 6.8 Illustration of the sensitivity analysis of 9 parameters based on the CE objective function for a sub-basin (C12D) of the Vaal River in South Africa.

If one of the flow metrics that form part of the regional constraints has been selected, the RSA can be used as a rapid check to identify how many members of

an output ensemble are non-behavioural. If a large number of members of an ensemble are rejected, it may be necessary to revisit some of the parameter estimation equations, the basin physical data that were used or the interpretation of these data. Figure 6.9 shows the results of an earlier attempt to constraint model outputs from A42B, a sub-basin of the Mokolo River basin, using the mean monthly flow metric. In this case 9286 members of the output ensemble (20 000) were above the upper prediction limit of the regional constraint of runoff ratio (Q/P) suggesting that some part of the parameter estimation process was not successful. The diagram suggests that excessive values of both FT and GW are the major cause (see the dark green graphs for both parameters in Figure 6.9).

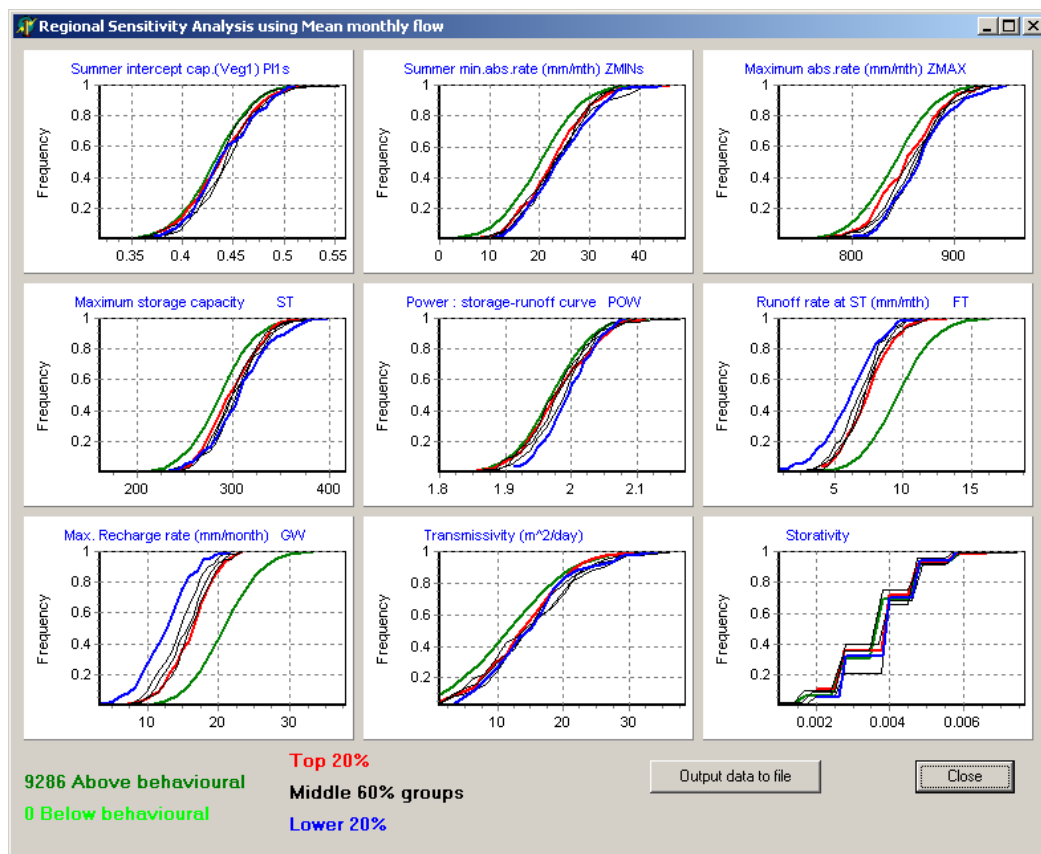


Figure 6.9 An illustration of how the additional information about the constraint is used to separate the behavioural from the non-behavioural ensemble members.

6.4 Summary

The efficient and, most importantly, consistent execution of the framework (Chapter 3) depends on the availability and/or development of appropriate software to support its implementation, otherwise it may be difficult to realise the intended goals. The main goal of the framework is to provide a consistent practical approach to model application that is capable of giving hydrologically plausible simulations in both gauged and ungauged basins of the region. Such an approach is expected to not only use the best knowledge available in the region but also to realistically incorporate the uncertainty in that knowledge. The tools discussed in this chapter relate to the generation of uncertain model parameter inputs, generation of ensembles from the population of all possible (or plausible) model outputs and assessments of the impact of the individual parameters on the results of the model. This section examined the development and use of these tools and explored how they are used in conjunction with each other to define and implement routine hydrological modeling strategies and/or objectives for sound scientific and practical application in water resources management.

The summary of the links between the tools is shown in Figure 6.10. This shows that the tools are part of an integrated system of hydrological modelling that can be used to store, manage, manipulate, analyse, present and interpret results. The tools occupy a niche within this system that enables uncertainties related to the parameterisation of the model to be accounted for and propagated through to the model output. Such information is necessary for practical use of models and modelling results especially when data scarce areas are being considered. A feedback loop, aimed correcting possible errors and improve utility of the tools, is also included within the execution of the tools.

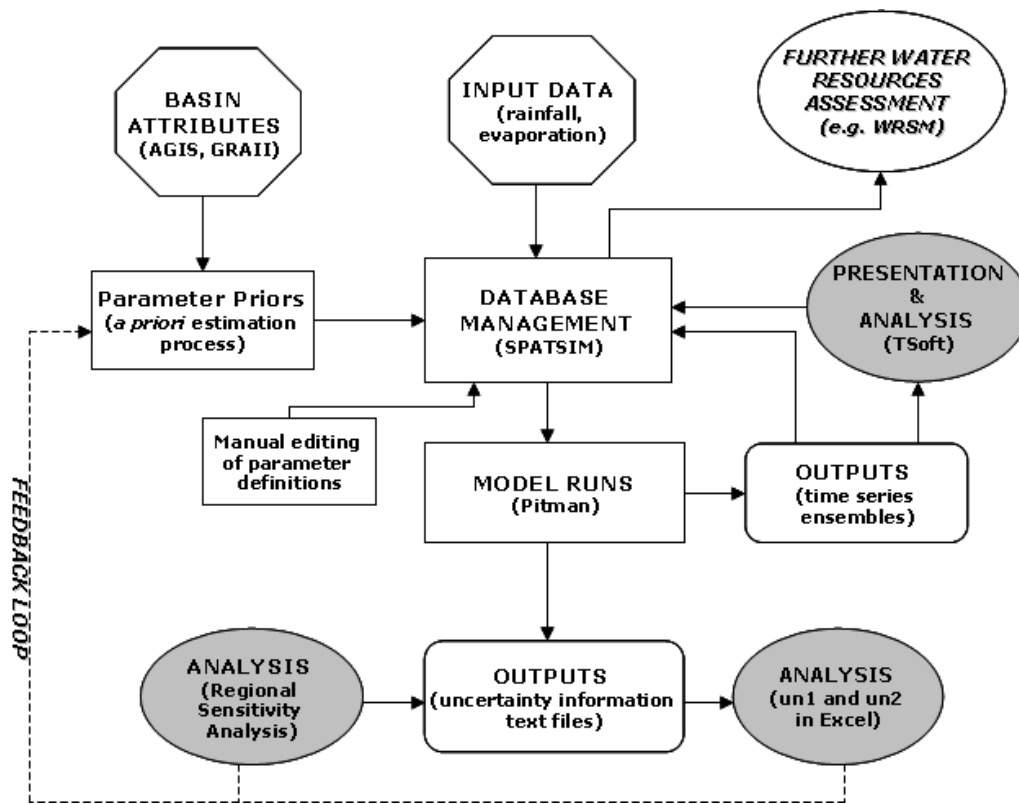


Figure 6.10 An illustration that summarises the linkages between the tools developed to implement the framework

The tools discussed in this chapter are practical and can be used with ease. The automation and packaging of the tools into a software package should make them manageable to use (with little training) by practitioners in the water sector. Use of the tools is envisaged to increase the chances of water practitioners taking actions consistent with current scientific norms and best practice in water resources planning. Such actions should also be consistent across different users within the same or similar systems. Their major strength lies in the fact that they are flexible and are useable with existing common water resources assessment tools that have been used for a long time within the region. This implies that practitioners are unlikely to resist their introduction as they are essentially an additional facility aimed at improving the tools they are familiar with and the manipulation and interpretation of results thereof. The use of the tools should, therefore, increase the reliability and confidence that can be expressed in the model results. The possibility of integration into SPATSIM means the management and storage of results can be done in a common database for ease of use. The tools are quite clear and robust enough to produce results that are not difficult to understand. They are used to achieve specific scientific and practical goals (i.e.

estimation of model parameters and their sensitivity analysis), important steps in assessing the hydrology of any given basin.

In the context of water resources management and decision making, the framework and the tools for its implementation represent a methodology for developing a common and consistent scientific development for effective decision making and outlining the process by which these will be made. The tools help to provide practical solutions to the problem of making predictions of hydrological fluxes in ungauged basins. The information that they produce is important for making these decisions with more confidence than is currently the case. If water managers or practitioners are aware of the limitations of their information or the uncertainties thereof, they will be cognizant of the risks attendant to the decisions that they will make. Thus, for the purposes for which they have been designed, the tools appear quite adequate. However, in order to realize the potential and value in these tools (and the framework), sufficient and credible data is required and this may require some investment. This is premised on the understanding the effectiveness of tools will be very much dependent on the extent to which the information available suits the needs of the management requirements and targets within any water resource management area.

CHAPTER 7

RESULTS AND DISCUSSION OF EXAMPLE APPLICATIONS

7.1 Introduction

This chapter presents the results of applying the various tools discussed in the preceding chapters with the Pitman model (Pitman, 1973). The tests were carried out using South African basins. While the whole point of taking the approach contained in this study is to use data on basin hydro-climatic and physical attributes that are relatively easily available within the region to estimate model parameters (Chapter 4) and constrain model outputs (Chapter 5), these data are not available throughout the region at the same resolution. South African data represent the best possible data available (in terms of both quantity and quality) and have been used to develop and test the applicability of the components of the framework (Chapter 3). Application in other parts of the region may require adjustment of the framework components to suit local data conditions. The results and discussion on the preliminary application of the framework, based on selected basins in South Africa, are presented. The results are a development of the earlier attempt at incorporating various sources of uncertainty into the Pitman model simulations by Hughes et al. (2008).

7.2 Description of example basins

There were 46 test basins used in this study and these were selected to span the possible ranges of hydro-climatic and geo-physical conditions obtaining in the country. Table 7.1a shows the hydro-climatic information of the selected basins, Table 7.1b summarises the ensemble results, while Table 7.1c shows the physical descriptions of some of the basins (note that the full list of basins is given in Appendix A). Table 7.1b includes the minimum and maximum of the simulated values of the three constraint variables. While observed stream flow data are available for 20 of the selected basins, the rest are ungauged. However, all the sub-basins are treated as ungauged in the parameter estimation process and tested against the constraints. Where the gauged data are available, these provide an additional test for the parameter estimation procedures. It should also be noted that most of the parameter PDFs are Normal and the uncertainty distributions of the output ensembles are therefore close to being normally

distributed as well. The ranges of the values given in Table 7.1b represent the tails of these distributions and a large number of the ensembles will lie within a narrower band.

The model was applied to all basins for the standard WR90 (Midgley et al., 1994) 70 year period from October 1920 to September 1990 using the WR90 rainfall data as inputs. This was necessary for purposes of comparison and drawing reasonable conclusions from the study without the influence exerted by the length of modelling period (Gorgens, 1984; Siebert and Beven, 2009). The time period used is long enough to be able to capture most of the expected hydrologic signals (low and high flows and extremes such as floods) observable in the region. The input data requirements to force the model (rainfall and evaporation demand) were assumed invariable and were taken from Midgley et al. (1994), while the parameters (and their feasible spaces) were estimated by the methods outlined in Chapter 4 and in Kapangaziwiri (2008) and Kapangaziwiri and Hughes (2008). While all parameters are capable of being applied with uncertainty, only the main runoff generation, moisture store, accounting and ground water accounting parameters were assessed for uncertainty. This was because these are the most critical parameters pertaining to natural hydrologic processes and most of those not considered account for human influences. Table 3.1 and Table 3.2 list all the Pitman (Pitman, 1973) model parameters and give brief descriptions. While the WR2005 (Bailey, 2009) data became available towards the end of this study, there was not enough time to pre-process these data. The results are not expected to be inconsistent with those derived from the WR90 study (Midgley et al., 1994). The WR2005 (Bailey, 2009) data are an update of the WR90 information (Midgley et al., 1994) adding 15 years to the time series of rainfall and river flow data. While there are changes in some components (e.g. changes in MAR or MAP), these are not substantial and were not expected to make a large difference to the results of the present study. However, pre-processing of the data has already started and will be used to update the results of this study in the longer term.

Table 7.1a A summary of the hydro-meteorological properties of the test basins.

Site	Region	P (mm)	PE (mm)	Area (km ²)	P/PE	Elev Range (m)	Obs. Q/P	Min GRAII	Mean GRAII	Max GRAII
								Mean annual recharge (mm)		
A42A	2	639.9	1700	573.4	0.376	113	U/G	10.16	33.88	55.61
A42B	2	659.9	1700	521.6	0.388	174	U/G	13.01	37.48	62.56
A42C	2	651.8	1700	1793.3	0.383	192	U/G	12.23	36.57	60.92
A42D	4	667.3	1700	496.6	0.393	139	0.202	15.16	39.64	66.85
A42E	4	639.7	1731	3297.2	0.37	157	U/G	7.2	28.85	46.04
A42F	3	624.9	1747	4318.8	0.358	110	U/G	7.2	27.89	44.68
A92A	4	831.2	1500	328.9	0.554	202	0.414	60.23	74.12	134.06
B41G	3	650.2	1500	149.5	0.433	302	0.143	27.11	47.68	83.73
C12D	2	666.9	1580	899	0.422	32	0.091	11.63	36.46	60.32
D55C	5	217	2150	760.4	0.101	78	U/G	0.75	7.22	10.09
G10E	5	639.9	1635	394.1	0.391	469	0.384	20.88	42.75	73.82
H10A	5	512.4	1670	233.7	0.307	393	U/G	11.17	30	50.43
H10B	5	707.8	1650	162.5	0.429	361	U/G	41.78	58.46	104.62
H10C	5	624.6	1650	655.7	0.379	428	0.292	22.85	45.74	79.23
J33C	4	292.9	2070	428.1	0.141	310	U/G	1.66	10.29	14.74
J33D	5	379	1980	258.9	0.191	415	U/G	4.7	17.94	28.58
K40A	4	705.6	1400	87.5	0.504	149	0.18	20.86	45.94	78.95
K40B	3	845.6	1400	111.6	0.604	201	0.175	34.93	61.99	108.85
M10B	4	557.5	1600	392.9	0.348	210	U/G	7.86	27.93	44.26
N24A	5	246.3	1950	665.8	0.126	67	U/G	0.24	5.83	6.54
Q14A	4	348.2	1850	485.7	0.188	178	U/G	5.57	18.47	30.33
Q14B	4	345.1	1850	725.3	0.187	229	U/G	5.53	18.13	29.68
Q92F	2	414.7	1650	665.3	0.251	232	U/G	0.61	10.6	12.7
R20A	2	1010.7	1450	139.4	0.697	209	0.255	32.4	67.31	116.18
R20B	2	844.9	1450	294.1	0.583	132	0.216	10.22	35.65	58.04
R20C	2	800.2	1450	121	0.552	152	0.161	14.45	43.63	72.15
R20D	2	733.1	1450	673.5	0.506	70	0.152	4.69	24.62	38.03
S60C	3	668.5	1500	215.8	0.446	202	0.127	15.23	39.89	67.33
T35C	3	916	1400	306.1	0.654	374	0.21	39.78	67.71	119.06
T40A	1	994.5	1200	208.1	0.829	251	U/G	109.46	126.36	203.08
T40B	1	979.4	1200	277.7	0.816	257	U/G	97.46	98.36	180.6
T40C	2	934.4	1200	722.9	0.779	132	0.273	87.79	95.01	162.19
U20A	2	1009.8	1300	293.3	0.777	210	U/G	51.83	79.94	142.13
U20B	1	987.8	1300	352.9	0.76	149	0.229	41.1	72.63	127.59
U20C	1	977.9	1285	925.1	0.761	159	U/G	35.43	66.33	115.87

V20A	2	1024.6	1300	267.1	0.788	201	0.383	61.67	85.4	153.01
V60A	2	891.1	1400	106.8	0.637	151	0.198	31.82	62.11	108.1
V60B	2	851.1	1500	659	0.567	166	0.155	29.77	58.88	102.34
V70D	2	810.8	1350	198.4	0.601	126	0.191	25.16	53.29	91.75
X11A	1	681.7	1450	671.7	0.47	32	U/G	25.4	48.14	83.99
X11B	1	714.2	1450	596.6	0.493	55	U/G	29.84	52.57	92.44
X11C	1	700.4	1450	1588	0.483	45	U/G	34.49	55.4	98.15
X21A	3	763.2	1400	264.9	0.545	198	U/G	36.43	58.88	104.26
X21B	3	730.9	1400	643.2	0.522	228	U/G	35.47	55.58	98.67
X21C	3	739.5	1400	954.3	0.528	270	U/G	36.95	58.88	104.39
X31A	2	1241.1	1400	174.0	0.887	307	0.370	100.86	115.88	210.88

Table 7.1b A summary of the ensemble results for the test basins.

Site	Min Q	Max Q	Min FDC	Max FDC	Min Rchg	Max Rchg
A42A	1.352	5.753	1.67	4.2	5.3	44.7
A42B	2.527	5.128	1.72	4.09	9.6	41.4
A42C	9.92	18.85	1.99	2.93	8.1	42.3
A42D	2.969	6.864	1.68	3.54	13.2	71.7
A42E	19.079	30.878	1.98	2.91	3.1	35.8
A42F	23.324	37.917	1.96	2.74	2.5	28.3
A92A	4.099	10.418	2.03	4.49	15.8	106.4
B41G	1.045	1.967	2.04	4.59	21	75.6
C12D	1.971	7.669	3.08	13.14	4.3	20.3
D55C	0.63	3.88	3.69	9.05	0	54.1
G10E	6.034	9.9	1.97	5.9	11.7	197.5
H10A	2.228	4.011	3.43	8.08	18.8	130
H10B	3.281	4.484	3.79	8.13	14.2	113.7
H10C	9.016	13.307	4.55	7.55	31.3	96
J33C	0.15	1.188	2.74	4.81	0	21.5
J33D	0.828	2.145	2.37	4.32	18.2	75
K40A	0.433	1.091	1.74	4.43	0	37.7
K40B	0.656	1.806	1.18	2.27	37.1	105.3
M10B	2.011	4.991	2.2	5.44	8	94
N24A	0.426	1.404	2.87	4.11	0	4.3
Q14A	0.372	2.385	2.99	4.91	0	40.6
Q14B	1.009	3.547	3.56	6.46	4.5	22.9
Q92F	0.531	2.953	2.9	9.93	0	50.4
R20A	1.953	4.989	1.78	4.57	18.5	165.3

R20B	3.219	7.425	1.87	4.34	0	110.4
R20C	0.908	2.749	1.73	9.01	0	111.9
R20D	4.879	12.924	2.02	3.53	0	67.7
S60C	0.745	1.712	1.58	3.23	13.5	52.4
T35C	3.307	5.182	1.32	2.28	64.2	123.8
T40A	4.97	6.515	1.42	2.53	146	219.8
T40B	4.392	6.196	1.44	2.68	101.5	147.1
T40C	14.39	17.094	1.5	2.14	120.7	171.4
U20A	4.437	7.266	1.76	3.89	57.6	129.7
U20B	4.567	8.091	1.57	3.69	48.5	113.7
U20C	14.425	19.681	1.99	3.16	14.5	123.8
V20A	6.585	11.417	2.14	3.39	61.1	188.8
V60A	0.842	2.247	2.36	5.85	34.1	111.1
V60B	4.494	8.496	1.92	3.16	34.4	89.7
V70D	1.594	3.128	1.39	2.32	34.4	91.7
X11A	2.237	5.908	1.73	2.94	27.1	80
X11B	2.785	6.583	1.81	2.97	33.1	82.4
X11C	8.822	13.937	1.88	2.77	41.7	108.7
X21A	2.226	4.291	1.81	4.88	49.9	125.2
X21B	5.470	8.540	1.62	4.37	44.6	110.2
X21C	8.680	12.395	1.69	3.94	43.9	111.4
X31A	5.647	7.585	1.68	3.04	141.5	221.4

Notes for Tables 7.1a and 7.1b:

- Region refers to the 'Budyko' region (see Figure 5.2)
- P and PE are mean annual precipitation and potential evaporation (mm/year).
- Simulated Q (Min and Max) represent the full range of the simulated mean monthly runoff volumes (10^6 m^3) for all 10 000 ensembles.
- U/G refers to ungauged basin.
- Elev. Range is the elevation range within the catchment (m).
- Simulated FDC (Min and Max) represent the full range of the simulated slopes of the annual flow duration curve (as defined in Section 5.2.2) for all 10 000 ensembles.
- The three mean annual recharge estimates from the GRAII database (Min, Mean and Max GRAII).
- Simulated Recharge (Min and Max) represent the full range of the simulated mean annual groundwater recharge (mm) for all 10 000 ensembles.

Table 7.1c Brief physical descriptions of a sample of the sub-basins assessed in this study.

Sub-basin	Gauge	Physical description
C12D	C2H004	Undulating topography, moderate to deep clayey soils, inter-bedded shales and sandstones.
G10E	G1H008	Steep topography, moderately deep, porous sandy loams with some impermeable lenses; unconsolidated sedimentary strata.
H10A H10B H10C	Ungauged Ungauged H1H003	Steep, moderately deep sandy loams; Karoo shales and sandstones.
K40A	K4H003	Steep topography, shallow to moderate loamy sands; fractured granite. Present day impacts of plantations.
R20A R20B R20C R20D	Ungauged Ungauged R2H006 ungauged	Undulating topography, moderate to deep sandy loams; fractured granites.
U20A U20B U20C	Ungauged U2H007 Ungauged	Undulating topography, moderate to deep clays; fractured sedimentary strata.
V20A	V2H005	Undulating to steep topography, moderate to deep clayey loams; Karoo shales, sandstones, grit and coal.
V70D	V7H012	Steep topography, moderate to deep, clayey soils; inter-bedded mudstones, shales and sandstones.
X31A	X3H001	Steep topography, moderately deep sandy clay loams; dolomites and limestone.

7.3 Constraint analysis of model output ensembles

The procedure followed for analysis was to compare the model output ensembles with the three constraints referred to in Chapter 5. For all the basins, each output ensemble consisted of 10 000 model simulation results and the output text file .un1 was used for this analysis. As stated in Chapter 5 the extent of the uncertainty associated with a constraint was defined by $\pm 95\%$ prediction limits of the regression equation between the constraint and its hydro-climatic and/or physical predictors (Figure 7.1). For each ensemble member, the value of the constraint was computed and the results of all output ensembles were compared with the three constraints:

- ❖ The volume constraint based on 95% prediction intervals for the regional relationships between P/PE (aridity index) and Q/P (runoff ratio), explained in Section 5.2.1.
- ❖ The gradient of the FDC constraint based on 95% prediction intervals for the relationship, explained in Section 5.2.2.
- ❖ The ranges of groundwater recharge estimates provided in the GRAII database (Section 5.2.3).

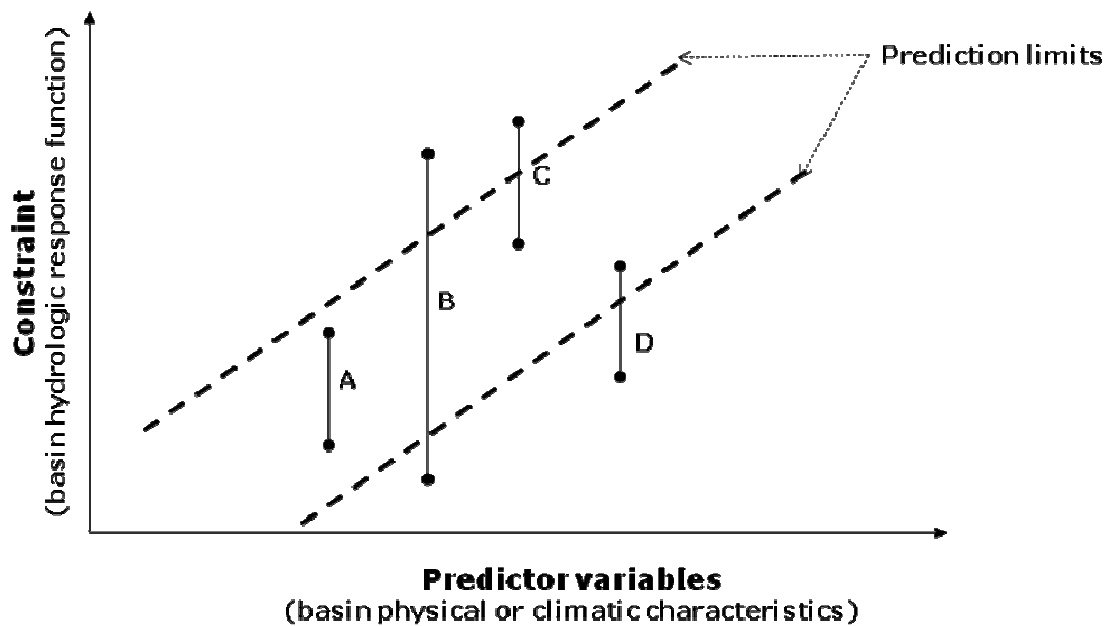


Figure 7.1 Illustration of the general constraint and predictor variables relationship used in this study. The analysis of model output ensembles produces the four possible outcomes (categories A to D).

There are a number of possible outcomes (or categories) associated with the process of constraining hydrologic response using the regionalized indices of hydrologic functional response characteristics (Figure 7.1). Category A represents the situation where the model output uncertainty is less than the uncertainty in the regional constraints, i.e. the range of variation of the output is within the constraint boundaries. This implies that the parameter estimation procedure has produced sets which generate acceptable outputs based on the metric of assessment, all the results are consistent with measured and expected hydrologic response and they are all behavioural (Beven and Binley, 1992; 2001). It should also be noted, however, that if the prediction limits of the constraints relationships are quite wide there would remain a high degree of uncertainty in the definition of behavioural response.

Category B is where the range of model ensemble results lies beyond both constraint limits (Figure 7.1). In this case, the constraint boundaries will determine the limits of acceptability of the model outputs. The ensemble members determined as non-behavioural (i.e. beyond the constraint limits) will

then be rejected. While this scenario indicates that some of the outputs are behavioural, the range of variation is too large and may indicate some latent problems either with the understanding or representation of the basin processes (e.g. presence of dolomites or large swamps/dambos), the applicability of the estimation procedure or the suitability/interpretation of available basin data. There are two possible courses of action in this situation. The first is that only those parameter sets giving results that fall within the regional constraints are accepted as behavioural and the model results generated by these parameter sets are used in any further analysis. This approach completely ignores the non-behavioural outputs and the parameter sets that produce them. The alternative is to identify (if possible) the part of the parameter estimation process that generates the non-behavioural results and use this information to re-assess the parameter estimation equations. While this approach has the potential to lead to an improvement in the parameter estimation process (and probably its credibility and robustness), it should be recognized that the degree of equifinality (Beven, 1993), and a frequent lack of identifiability of the parameters of the Pitman model may make this approach ineffective.

Categories C and D are where the range of variability in the model outputs is predominantly above (or below) the upper (or lower) constraint boundary (Figure 7.1). This indicates a bias towards either over- or under-simulation in the model output ensembles. Extreme examples of C and D occur when none of the outputs lie within the constraint limits. Such scenarios may indicate inconsistency between the model and the constraints and, therefore, demand an investigation of the parameter estimation or the constraint development processes. The case where all the outputs are outside the constraint boundaries is a cause for concern because it may suggest a complete failure of the parameter estimation process. However, it may also point to the importance of other sources of uncertainty such as the input data (rainfall and evaporation demand), or model structure errors, which are not considered here. The most logical action would therefore be to first examine and ascertain the validity and/or representativeness of the input data. This is especially important where the ability to define catchment scale estimates of the inputs is not ideal and the most common problem is the definition of rainfall inputs in mountainous areas where rainfall measurement networks are usually sparse. Invalid and biased forcing data inevitably result in biased and/or erroneous simulations which may only be detected when compared with the constraints. In a modelling approach that is based on calibration, the parameter values implicitly account for the inadequacies in the input hydro-meteorological

data (Andreassian et al., 2001). The same is not true where an *a priori* parameter estimation approach is used.

The second step would be to interrogate the outputs in detail (see section 7.5 on sensitivity analysis) to identify where the parameter estimation process produces non-behavioural results and to question the interpretation of the catchment property data. In many cases during the initial testing of these methods, this approach yielded improved results especially when carried out in a structured manner by looking at the different components of the model (surface runoff generation, unsaturated zone runoff and ground water recharge) separately. The interpretation of the input basin physical data can account for some errors, and the main problem occurs with the subjectivity of the interpretation process when the spatial variability within a basin is large. The variability in the basin physical data and the subjectivity in its interpretation are closely linked to the scale of model application. However, if there are no problems with the input hydro-meteorological data and the interpretation of the physical property data is realistic, it may be necessary to accept that the parameter estimation equations (and, possibly the model structure) are not suited to the specific catchment.

In the present study, the approach discussed in the last few paragraphs has been applied only to the volume (runoff ratio) and the FDC slope constraints since the ground water recharge constraint is not constructed in same manner. The runoff ratio relationships are regionalized while the FDC slope is currently applied at the national scale.

7.3.1 Volume constraint: Runoff-ratio (Q/P)

For regions 1 to 5, there were 7, 16, 8, 8 and 7 basins respectively (Table 7.1). Figures 7.2 to 7.6 illustrate the comparisons between the output ensembles and the regionalized mean annual volume constraint (using Q/P). For clarity, region 2 is presented using two diagrams (Figure 7.3 a and b). Table 7.2 shows the basis used for the determination of category A, C and D candidates. It was realized that with some sub-basins displaying only few outputs beyond constraint boundaries, it would be logical to have these sub-basins in A rather than either C or D. Results were classified as category A if only 10% or less of the outputs were beyond the constraint limits. This cutoff point was chosen arbitrarily but seems reasonable as it limits the variability to an acceptable level. The final results are summarized in Table 7.3.

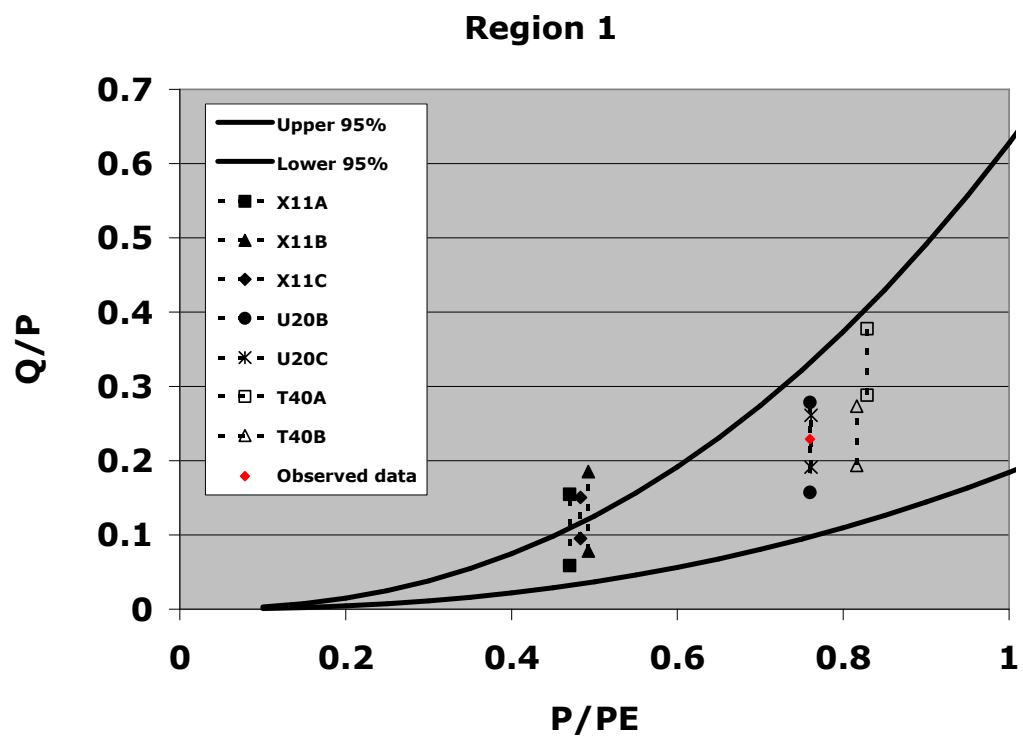


Figure 7.2 95% prediction intervals for the P/PE v Q/P relationship for Region 1 compared with the range of output ensembles.

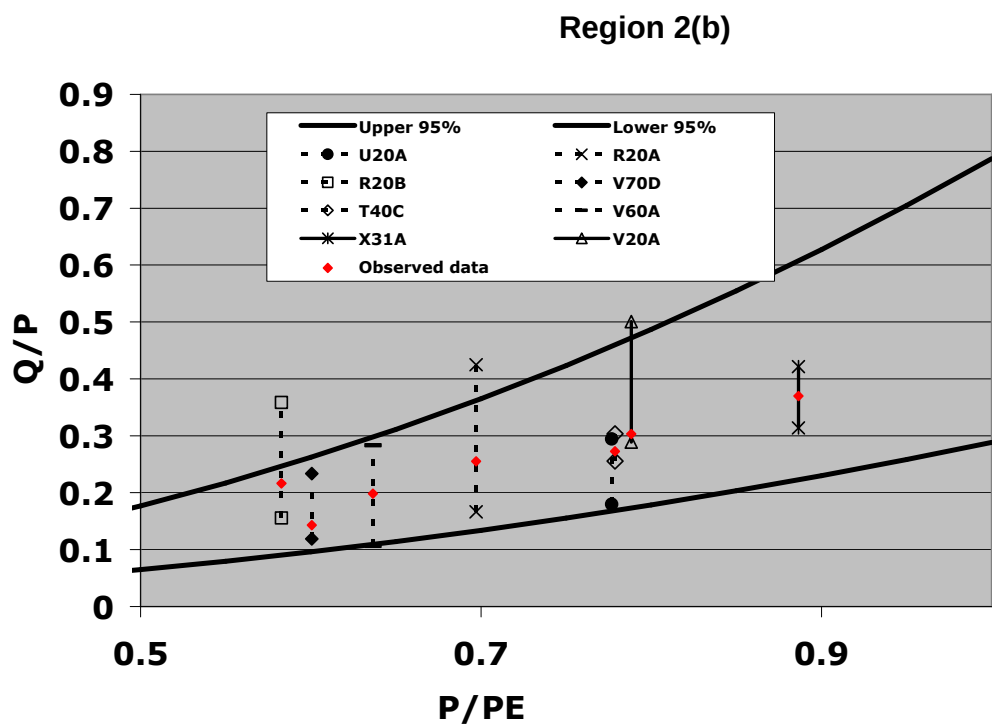
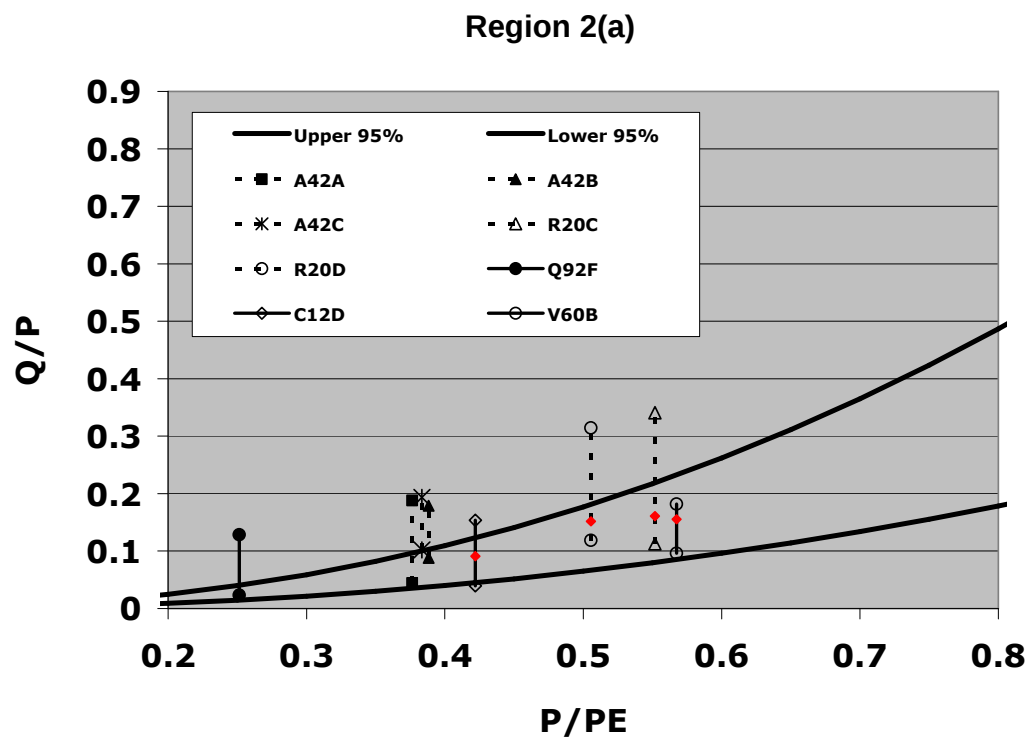


Figure 7.3 95% prediction intervals for the P/PE v Q/P relationship for Region 2 compared with the range of output ensembles.

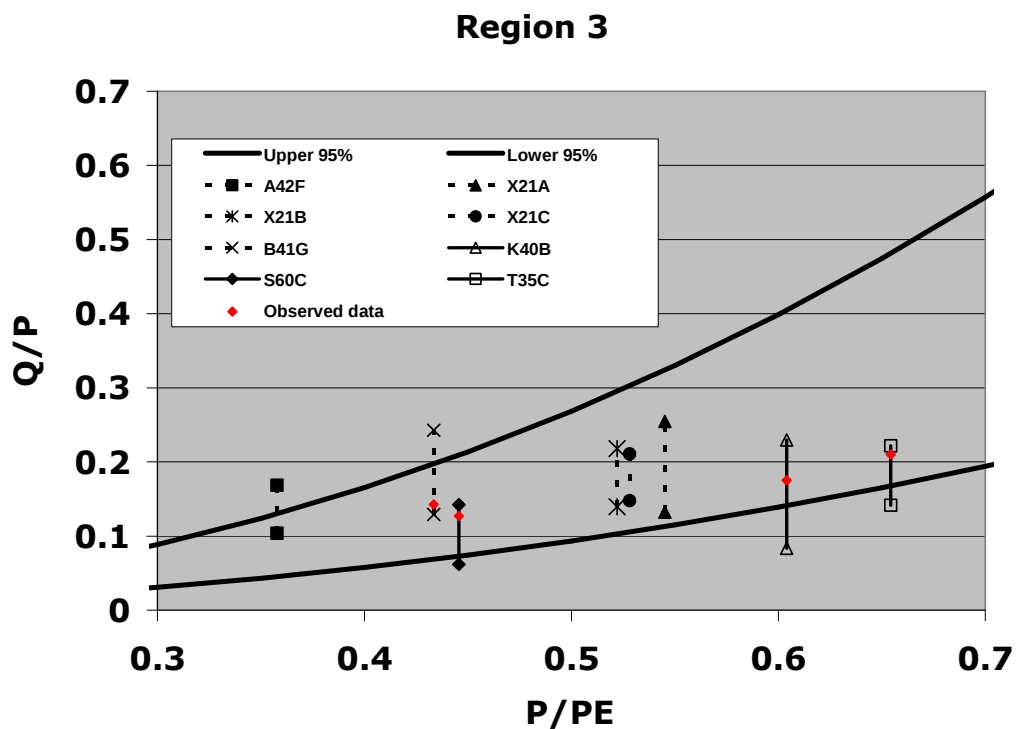


Figure 7.4 95% prediction intervals for the P/PE v Q/P relationship for Region 3 compared with the range of output ensembles.

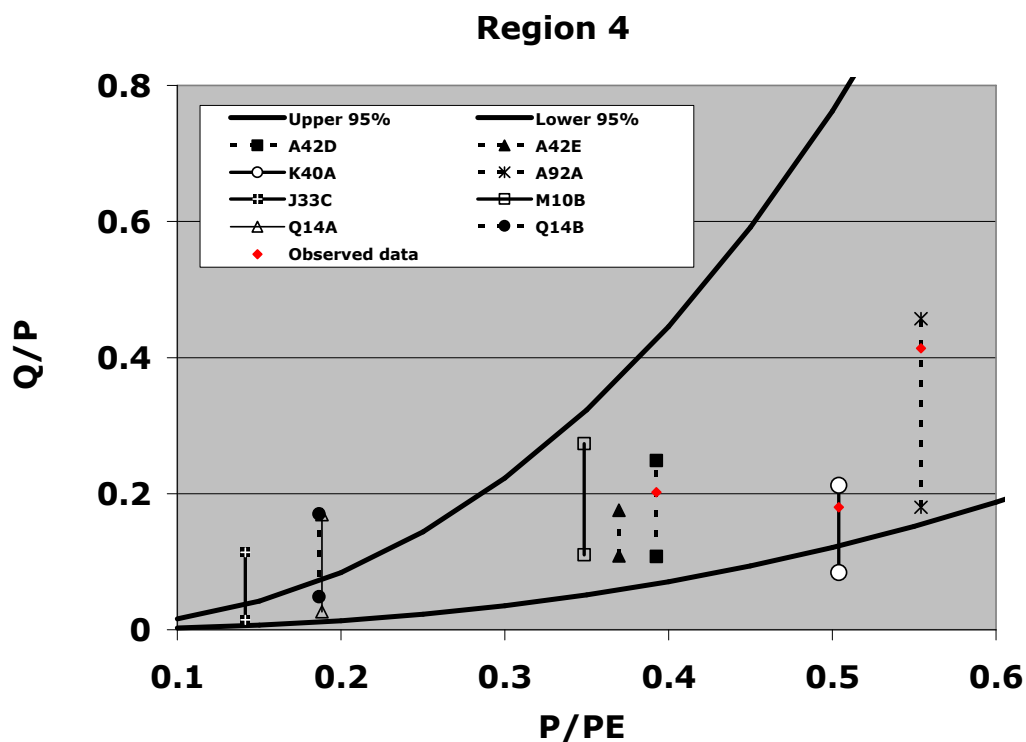


Figure 7.5 95% prediction intervals for the P/PE v Q/P relationship for Region 4 compared with the range of output ensembles.

Region 5

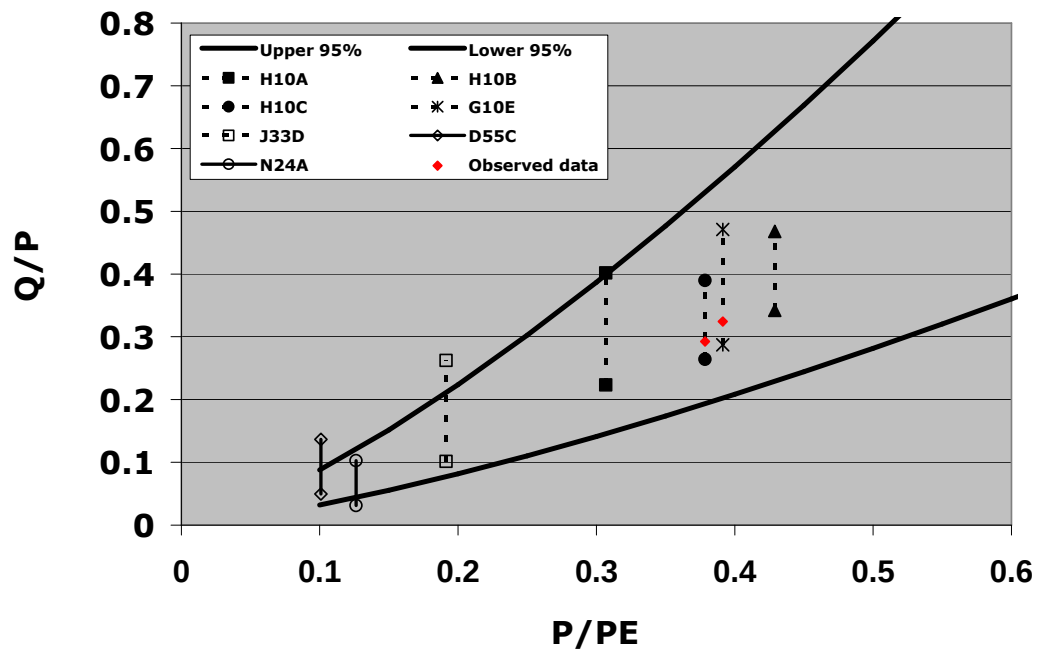


Figure 7.6 95% prediction intervals for the P/PE v Q/P relationship for Region 5 compared with the range of output ensembles.

Table 7.2 Analysis of outputs to determine candidates for categories A, C and D. Possible causes of the non-behavioural outputs is given in column 5. SD refers to standard deviation and the value of the standard deviation relative to the mean is given in brackets.

Region	Basin	% Above constraint	% Below constraint	Possible explanation	Final Category
1	X11A	22.37	0.00		C
	X11B	80.67	0.00	High ZMIN SD (37%)	C
	X11C	87.81	0.00	High ZMIN SD (40%)	C
2	A42A	65.66	0.00	High FT SD (50%)	C
	A42B	92.78	0.00	High ZMIN SD (31%)	C
	A42C	99.46	0.00	High ZMIN SD (30%)	C
	C12D	11.37	1.09		C
	Q92F	98.99	0.00	High ZMIN SD (33%)	C
	R20A	4.94	0.00		A
	R20B	93.97	0.00	High ZMIN SD (90%)	C
	R20C	72.74	0.00	High ZMIN SD (50%)	C
	R20D	62.51	0.00	High ZMIN SD (93%)	C
	V20A	0.51	0.00		A
3	A42F	76.56	0.00	High ZMIN SD (38%)	C
	B41G	22.02	0.00		C
	K40B	0.00	1.99		A
	S60C	0.00	0.21		A
	T35C	0.00	15.05		D
4	J33C	94.62	0.00	High FT SD (27%)	C
	K40A	0.00	9.20		A
	Q14A	93.42	0.00	High ZMIN SD (40%)	C
	Q14B	95.42	0.00	High ZMIN SD (48%)	C
5	D55C	97.54	0.00	High ZMIN SD (35%)	C
	H10A	1.65	0.00		A
	J33D	5.78	0.00		A
	N24A	0.00	1.23		A

Table 7.3 Summary of the results of the frequency of occurrence of categories A to D in the comparison of the model output ensembles with the volume constraint. The values are the percentage number of catchments within each region falling into the different categories.

Region	No. in region	Possible scenarios			
		A	B	C	D
Description		Low parameter uncertainty	Excessive parameter uncertainty	Parameters giving outputs above limit	Parameters giving outputs below limit
Runoff ratio constraint					
Region 1	7	50%	25%	13%	0%
Region 2	16	44%	31%	25%	0%
Region 3	8	63%	0%	25%	13%
Region 4	8	63%	38%	0%	0%
Region 5	7	86%	14%	0%	0%
Total	46	59%	24%	15%	2%
FDC slope constraint					
All regions	46	31%	2%	2%	65%

Table 7.3 shows that for the runoff ratio constraint the results are generally acceptable and that the model output ensembles are frequently within expected ranges of constraint uncertainty. Only 2% of the basins produced excessive and unacceptable parameter uncertainty. In Table 7.3 category B includes those basins whose ensemble ranges were large irrespective of whether or not the ranges extended beyond (for at least 80% of the outputs) both constraint limits, e.g. Q14A and J33C (Figure 7.5). Categories C and D included those ensembles whose ranges of variability were lower than the B category but included outputs that extended either above (category C) or below (category D) the constraint limit. One of the key observations is that the ensemble ranges tended to extend beyond the upper constraint limit rather than the lower one (e.g. X11A-C in Region 1, V20A and R20D in Region 2, A42F in Region 3, Q14A in Region 4 and J33D in Region 5). This is the result of over-simulation of the mean volume. The implication is that there could be a systematic error in one or more components of the parameter estimation procedure. There is only one basin (C12D, Region 2) that extends beyond both the lower and upper limits of the regional constraint, while A42A (Region 2), J33C (Region 4) and D55C (Region 5) come quite close. Another observation is that the range of variability exhibited by some of the ensembles (e.g. R20C in Region 2), even where the ensembles are within the constraint limits (e.g. A92A in Region 4), is quite large. It should be noted that at high P/PE values the constraint uncertainty is quite high, and associated with the logarithmic form of the constraint prediction relationship. It is important to stress

that this magnitude of uncertainty may make model-reliant water resources decision making difficult.

An examination of the topography (through Google Earth for example) and/or the land types of some of the problem sub-basins revealed large variabilities within the basins in terms of the topography and/or land types. Such sub-basins as H10A-C, A42A-C, R20A-D, C12D and K40A exhibited these variations and this may have led to a possible miss-interpretation of the basin physical property data. In such cases the lumped estimation process of the basin physical attributes leads to higher levels of uncertainty. Related to this is the scale issue, where the mismatch between the scales of model application and the physical basin data lead to more uncertain parameters. The impacts are investigated later in section 7.4.

In spite of the problems outlined in the previous paragraph, there are many catchments in the example set where the ensemble results are either within (category A, 27 out of 46) the range of regional constraints or not excessively outside this range (categories C and D, 8 out of 46). Thus, the parameter estimation procedures seem to be relatively successful for the group of basins studied, where success is measured against the regional runoff-ratio metric. In the majority of the remaining sub-basins where the uncertainty is large or the results are heavily biased (11 out of 46), a sizeable proportion of the ensembles are within the regional constraint values, suggesting that the focus of any improvement in the parameter estimation process should be on the outlier parameter sets. Many of the naturalized observed streamflow data points (section 5.2.1) are located close to the middle of the range of the output ensembles. This supports the observation that the variance of the parameter uncertainty distributions rather than the mean (or best estimate) values requires further investigation. Figure 7.7 is an illustration of the location of the historical observations on the frequency cumulative curve for the ensemble of some of the sub-basins.

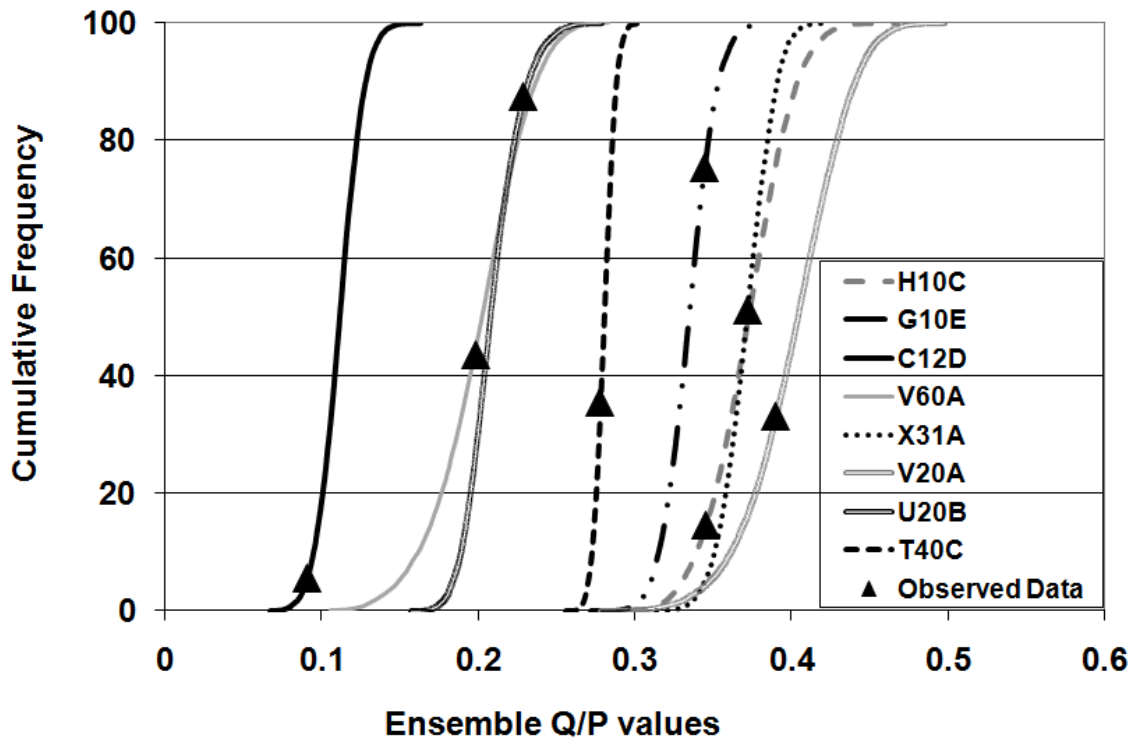


Figure 7.7 Cumulative frequency distribution of the Q/P values for the output ensembles compared with observed data values (represented by the black triangles).

Figure 7.7 can be used to gauge the success of the parameter estimation process in a gauged sub-basin. The ideal situation is to have the observed data lying near the centre of the distribution. If it lies at or near the tail-ends of the distribution then it is either a problem with the data or the estimation of the parameter priors. The former is illustrated in the sub-basin H10C where the observed data is close to the lower end of the distribution, implying that about 94% of the simulations are above the observed point. However, a close examination of the WR90 (Midgley et al., 1994) database reveals that the naturalized and patched observed flow data are almost identical. This is worrying as it implies no upstream developments in the sub-basin when in fact there are a large number of farm dams (Hughes and Mantel, 2010). Thus, the naturalized observed flows obtained from WR90 are an under-estimate of the expected natural flows in the sub-basin. This clearly illustrates the hazards associated with using historical data and the naturalization process. The point is that in many cases the upstream developments and water-use are often unknown or poorly quantified. C12D represents an example of bias in the ensembles relative to observed data which was later identified as being related to the interpretation of the physical property

data. Section 7.4 discusses the effects of scale and the bias for C12D was reduced by applying the parameter estimation process at a smaller scale.

In Table 7.2 (or Figures 7.2 to 7.6) there are 15 basins where more than 60% of the ensembles extend beyond the constraint limits (categories C and D). Further analysis reveals that, except for A42A and J33C, the variability of parameter ZMIN is quite high, from about 30% of the mean (for A42B and A42C) to 90% and 93% for R20B and R20D respectively. This observation can be explained in terms of the variability of the basin soil characteristics, whose distribution properties are used to determine the uncertainty of the infiltration parameters. However, it is surprising that the variability of parameter ZMAX is not equally high, and is less than 10% of the mean for all basins. The variability in the other basins (A42A and J33C) seems to be influenced by the large standard deviations of the parameter FT. In all cases, it was found that the distribution types were Normal, and that the output variability was not caused by highly skewed input parameter distributions.

The uncertainty version of the Pitman model allows for the setting of minimum and maximum parameter values. In this study these were only set to prevent parameter values that are structurally impossible (e.g. negative parameter values). Thus, the sampling process from the Normal (or occasionally Log-Normal) parameter distributions was effectively unconstrained. However, in situations where no estimation equation is available for a parameter a Uniform distribution is commonly used and setting the minimum and maximum parameter to define a sensible range becomes an important consideration. This situation would apply if some of the water use parameters were to be included as part of the uncertainty analysis.

7.3.2 Gradient of the monthly Flow Duration Curve (FDC)

Figure 7.8 illustrates the comparisons between the ensemble outputs and the constraints for the gradient of the monthly FDC. Table 7.3 lists the frequencies of the basins that fall into the categories A to D. 31% (14 out of 46) of the basins exhibit FDC ensembles that lie within the constraint limits or slightly outside (less than 10% of ensembles) the limits indicating that there is low uncertainty and almost all of the outputs are behavioural (scenario A). Only one basin, R20C, can be classified as category B where the ensemble range extends beyond both constraint boundaries and the uncertainty is excessive and unacceptable.

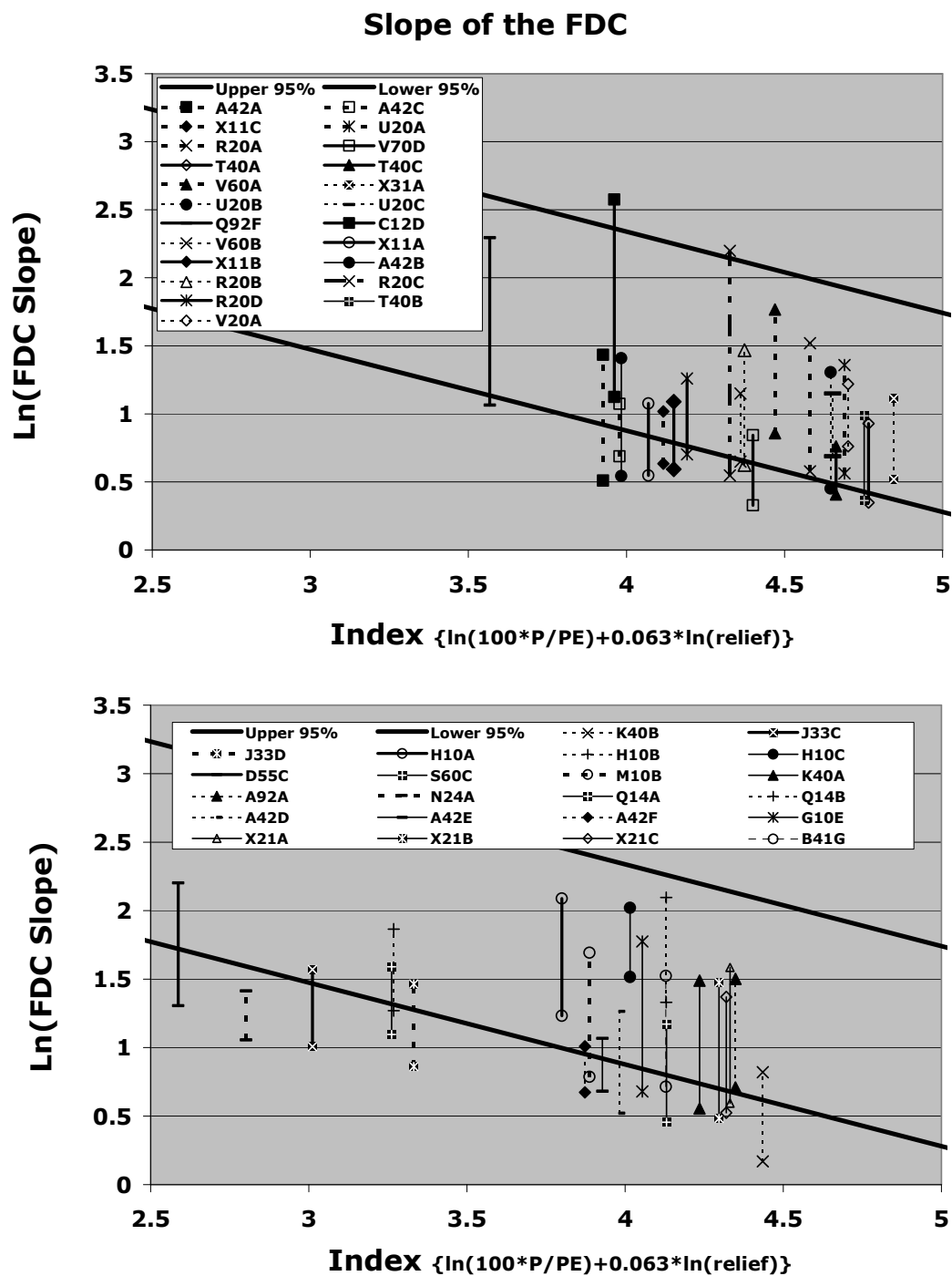


Figure 7.8 95% confidence intervals for the flow duration curve relationship compared with the range of ensemble outputs.

The general tendency is for ensemble FDC slopes to be lower than the constraint boundary (category D rather than C) suggesting that the ensembles are generating excessive low flows. There is only one basin (R20C) whose ensemble ranges of FDC slopes extends beyond the upper limit (scenario C). The basins

that have some non-behavioural outputs based on the volume constraint also exhibit problems using the FDC slope criterion (e.g. K40A, K40B, T35C, C12D, R20C, Q14B, N24A and S60C). For instance, K40B, J33C and J33D have low FDC slopes for the majority of the ensembles as well as many non-behavioural volume ensembles. The ensembles for all the sub-basins R20A-D, A42A-C and Q14A-B seem to generate low FDC slopes as well as generally over-simulating the volume. One possible explanation of this occurrence is that there is a high degree of uncertainty in the values of those model parameters that generate runoff (e.g. ZMIN, ZMAX, FT and POW). The large standard deviations of the ZMIN and FT parameters were highlighted earlier. However, a closer examination of the overall simulations shows that the parameters seemed to properly capture the variability of the hydrologic regime of the various basins (some example plots are shown in Appendix D).

There appears to be a complete failure in the case of basin N24A whose outputs all lay outside the lower constraint boundary. This is surprising given that the volumes simulated for the basin have low uncertainty with only a very small proportion of the outputs lying beyond the lower volume constraint boundary. What is also difficult to understand is that the basin is only covered by one land type which means there is little variation in the basin physical property data. N24A is a dry basin and has a high proportion of zero flows, while Figure 7.9 clearly shows that excessive recharge is not to blame, suggesting that other factors or sources of uncertainty may be more important than parameter uncertainty in this basin. The other dry basins (D55C, Q14A-B, and J33C-D) display a similar trend though they are not as severe as N24A. However, the general trend is towards lower slopes even in situations where the simulated volumes were behavioural. Even in the cases where the FDC slopes are behavioural, the observation has been that they are almost always closer to the lower, rather than the upper, limit of the constraint. A detailed examination of the ensembles reveals that in many of these basins there are instances where non-zero 90% FDC values are related to some extreme FT values which are unlikely to be behavioural (e.g. in R20D). Another possible explanation is that the high flows are generally being poorly simulated by the model. It could also be because the FDC slope calculation is quite sensitive to the number of zero flow months and perhaps this suggests that an additional constraint is required for the more arid basins where flow is not permanent. It would be worth exploring in future work the effects of changing the estimation equation for the FDC slope by using only time steps with flows greater than zero. One of the possible causes of low FDC

slopes in the ensembles is the excessive simulation of the low flows which could result from excessive groundwater recharge. This point is addressed in the next section.

7.3.3 Ground water recharge constraint

Figure 7.9 illustrates the comparisons between the three GRAII (DWAF, 2005) groundwater recharge estimates and the range (minimum and maximum) of the ensemble outputs. There are two quite clear conclusions that can be drawn from Figure 7.9. The first is that a high proportion (25 out of 46) of the minimum output ensembles are less than the lowest GRAII estimates of recharge and the second is that almost half (22 out of 46) of the maximum output ensembles are higher than the maximum GRAII estimates. There are 10 basins (including T35C, X31A, U20A, U20B, V60B and S60C) where the all the output ensembles are within the GRAII range and are therefore considered behavioural. The highest simulated annual ground water recharge values were 221.4 mm (X21C) and 219.8 mm (T40A) and the lowest was zero for eight basins including Q92F, D55C and J33C. The latter group consists of basins that are all in the drier regions of the country. While zero recharge is not likely to be a behavioural result these will have little effect on the simulations because no ground water discharges are expected in such areas.

One of the issues that the study had to take into account is the significance of the three recharge values in the GRAII database (DWAF, 2005). Firstly, the GRAII values are based on different methods and the extent to which these can represent uncertainty in the real recharge depends on the validity of the methods which is difficult to assess without more observed recharge data. Secondly, experience using the GRAII data suggests that the highest recharge values are not appropriate in many situations. Detailed analysis of model outputs in several sub-basins suggests that such high recharge values result in excessive low flows compared to observed streamflow data (Hughes and Parsons, 2005). However, in spite of the potential problems with the high recharge estimations from GRAII, they have been retained in this study as they can be considered to represent the extreme upper limit of recharge and are therefore useful to constrain the model outputs. One of the observations from Figure 7.9 is that, notwithstanding the recognized inadequacies in the estimation equation for the recharge parameter (see section 7.3.4), the uncertainty is not large in almost all the basins. The exceptions are G10E, H10A, H10B, M10B, A92A, R20A and V20A.

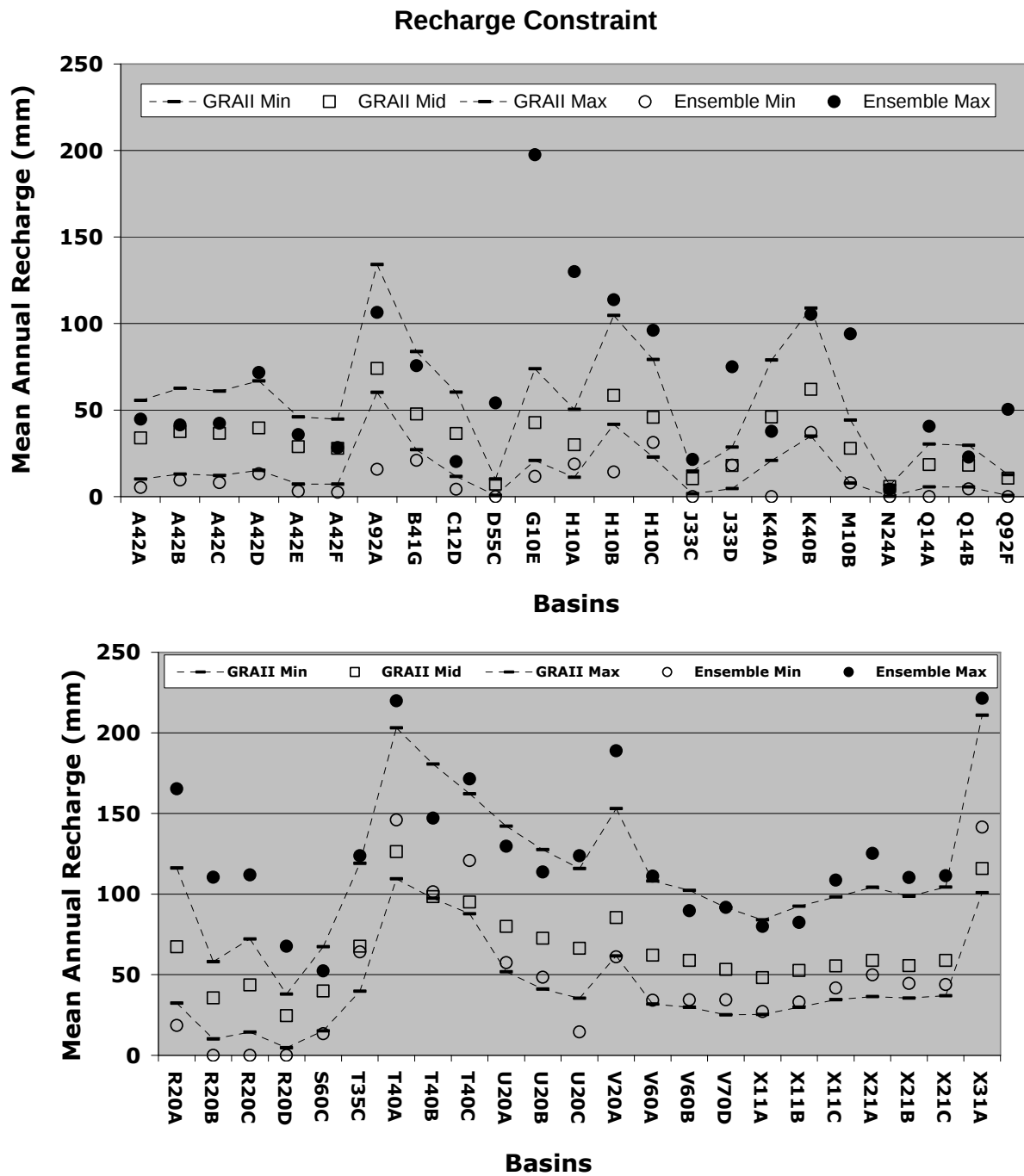


Figure 7.9 Comparisons between the three GRAII recharge estimates and the minimum and maximum recharge output ensemble estimates.

7.3.4 Calibrating parameter GW against the recharge constraint

The results for the simulated recharge (Figure 7.9) suggest possible problems with the estimation procedure for parameter GW. In the initial stages of the

establishment and evaluation of the framework, the ground water recharge constraint was applied to the ensembles in order to remove all the values higher than the maximum and lower than the minimum recharge estimates given in the GRAII database (DWAF, 2005). While the effect was generally negligible in most basins, there were some basins where the number of outputs rejected was high (e.g. initial tests with H10C and G10E resulted in 1695 and 4594 out of 5000 ensembles respectively being rejected). This initial evaluation revealed a number of problems with the recharge parameter estimation methods that resulted in excessive recharge values that were conceptually impossible and therefore resulted in excessive runoff volumes. An examination of the model structure revealed that in most of these cases, the model simulated more recharge output from the subsurface store than was available (a water balance error). This structural error was addressed by restricting the total value of the two subsurface moisture loss parameters (FT and GW) to be limited by the maximum subsurface moisture storage (ST). This change in the model resulted in much more realistic ranges of recharge estimates. The correction to the model code solves the water balance by rejecting excessive recharge values, but does not solve the problem of properly estimating the parameter GW. It is therefore imperative to not only correct the model code, but also to address this issue in the parameter estimation process and the parameter sampling procedure. This is an example of the feedback loop that was referred to during the presentation of the framework in Chapter 3.

Efforts to improve the estimation for parameter GW were not entirely successful. One of the problems in the original approach was that the distribution was almost always log-Normal with quite large standard deviation values. This resulted in a small number of excessively high GW values. The improved estimation approach removed this problem but there remain many basins where the recharge estimates are substantially greater than the constraints (Figure 7.9.). The process that has been followed is to manually adjust (calibrate) the GW parameter PDF (mean and standard deviation) to achieve an uncertainty range of the annual recharge that is close to the constraint limits (Figure 7.9) suggested by the GRAII data. The results of this process are illustrated in Figures 7.10 and 7.11 and Appendix B shows the calibrated distributions of GW for the test basins. The results of the overall simulations have improved and the uncertainty ranges for both the volume and FDC slope constraints are smaller and most outputs are behavioural. The reduction in the ranges resulted in most of the basins moving into category A, with low parameter uncertainty, though some basins continue to

have ensemble outputs outside the constraint boundaries. In such circumstances, there are other factors that may be important in determining the final model outputs such as scale and interpretation of land type data.

This calibration approach showed that the parameter GW had a huge influence on the outcome of the modelling process and the final results are acceptable. One of the advantages of this approach is that it can be used to condition and constrain model simulations in both gauged and ungauged basins given that the calibration is against the constraint, rather than observed data. This approach means that refining the GW parameter estimation is not a priority as the GRAII data constraints can be used instead. In any case, calibrating the GW parameter to the GRAII constraints is necessary in only limited circumstances where the current estimation equation fails.

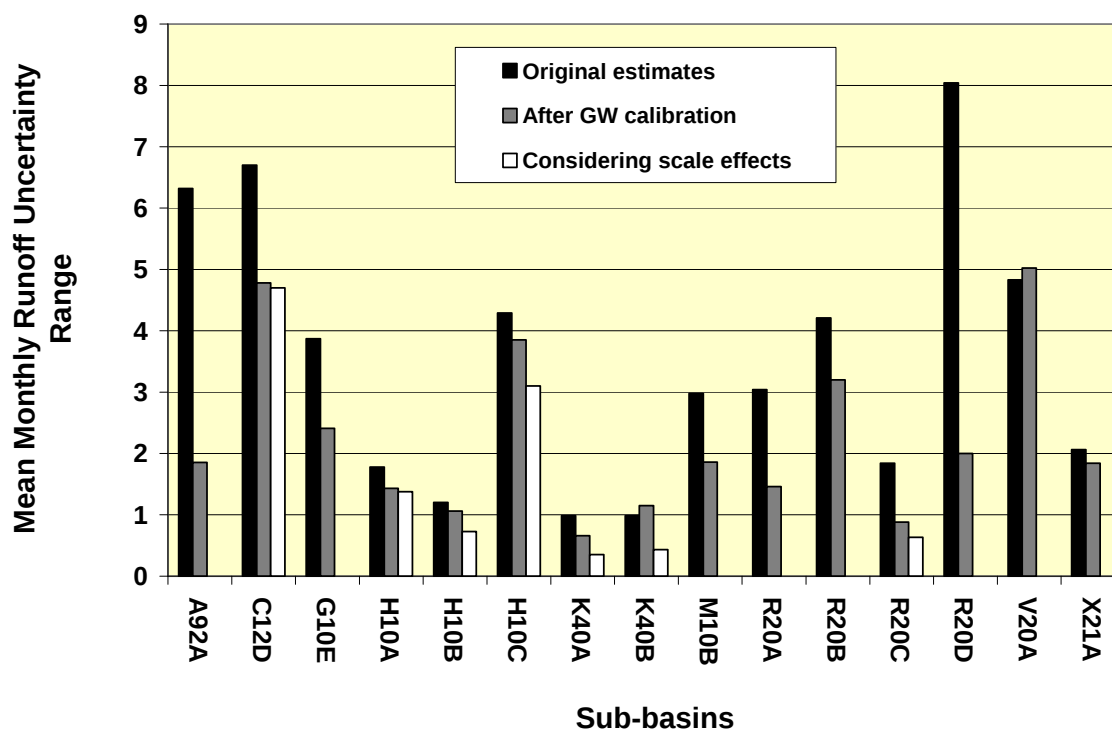


Figure 7.10 The impact of changes made to reduce parameter uncertainty analysed through the variation in the range of mean monthly flows (Mm^3).

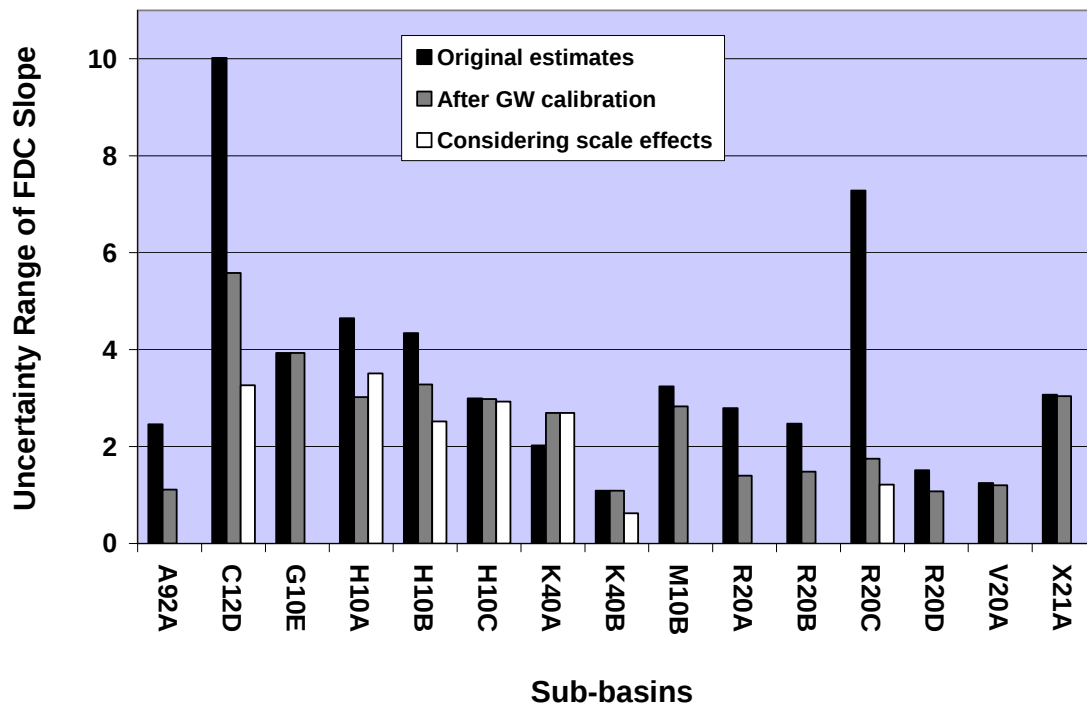


Figure 7.11 The impact of various changes made to reduce parameter uncertainty analysed through the variation in the range of FDC slopes.

7.4 Exploring the effects of scale on uncertainty

Besides the apparent problem in the estimation equation of parameter GW in influencing uncertainty ranges, two other issues also raised in the preceding discussions are the interpretation of the physical basin data and the scale of model application and parameter estimation. These issues are closely related and can be resolved by the same modification to the parameter estimation approach. It was highlighted that the issue of subjectivity in the interpretation of basin data is usually encountered when there is large variability in the data as a result of the occurrence of several land types and/or soil types within a sub-basin. In the current application of the model and parameter estimation process, these effects are lumped at the sub-basin scale to define distributions for the relevant basin physical properties. This section analyses the impacts of unbundling the physical properties estimation process using a smaller scale of model application and parameter estimation. The first step was to assess the subdivisions that could possibly be used for this exercise. In South Africa, there is an existing subdivision of the quaternary basins (the sub-basins at which scale the model is used

currently) into smaller so-called quaternaries (Schulze et al., 2007). However, while this approach results in smaller basins, these subdivisions do not, in most cases, coincide with the land type boundaries and using them would not have solved the problem. As a result, the subdivision of quaternary sub-basins was based on the interpretation of the land type data. This approach effectively groups areas dependent on their physical characteristics e.g. the higher, steeper, headwater areas with shallower soils were separated from lower, flatter areas with deeper soils. A nodal approach was adopted to investigate the scale effects. However, care had to be taken to realistically represent the variation of land type data without creating an excessive number of nodes. This approach achieves the objective of reducing subjectivity in the interpretation of the physical data and consequently, uncertainty in the estimation of the basin properties. Figure 7.12 and Figure 7.13 illustrate the variability of land type data in the Breede sub-basins (H10A-C) and the sub-basin (K40B).

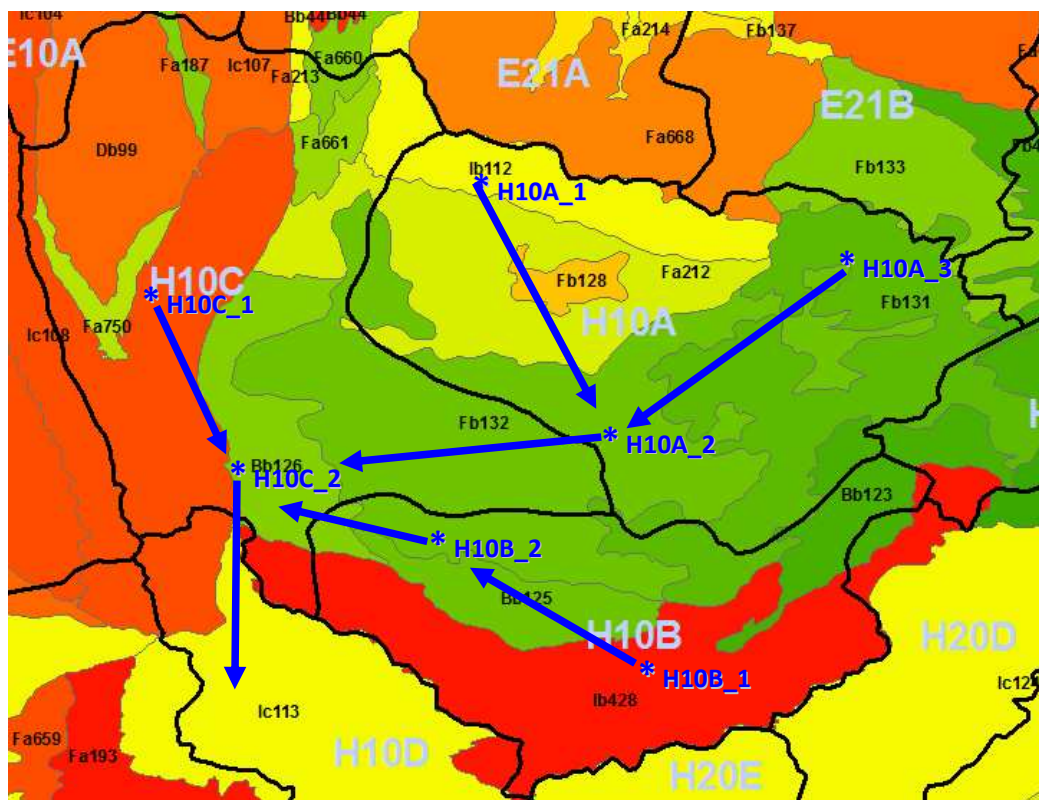


Figure 7.12 Illustration of the land type variation in sub-basins H10A-C. The nodes used are labeled and the arrows show the direction of flow.

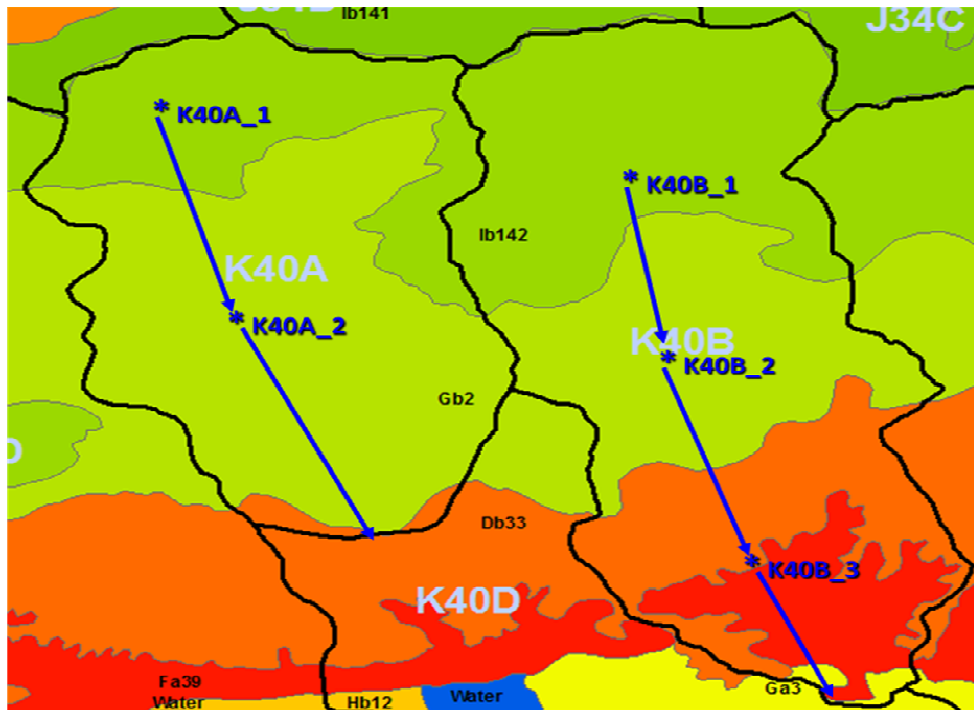


Figure 7.13 Illustration of the land type variation in the sub-basins (K40A-B) of Diep and Hoekraal River systems.

For the Breede system, H10A was divided into three sub-basins (H10A_1 to H10A_3), to represent the three distinct topographic units in the sub-basins. H10A_1 represents the high rugged terrain of the scarp faced areas. This includes the steeper components of the land types Ib112, Fb128 and Fa212. These components make up most of the top and mid slopes with no bottom or valley slope aspects. H10A_3 represents the steep slopes, mostly also top, mid slopes and some bottom slopes, of the land types Fb131 and Bb123. H10A_2 represents the low lying, bottom slopes and the valley and is dominated by the land type Fb132. For H10A, the arrangement is such that H10A_1 and H10A_3 would flow into the bottom subdivision, H10A_2. A similar approach was used to subdivide H10B and H10C into two sub-systems each, with the same notation as used for H10A. The outlets of the subdivisions for these sub-basins were at H10B_2 and H10C_2 respectively. H10A_2 and H10B_2 flow into H10C_2. What also needs to be noted is that the subdivisions also require a conceptualisation and interpretation of the recharge estimation based on the understanding that the steeper areas would be the recharge zones and the low lying areas the discharge zones. The GW parameter is adjusted to reflect this conceptualisation and understanding. The same understanding needs also to be extended to the parameters related to the drainage density (DDENS), riparian strip factor (RSF)

and the regional ground water slope (GWSlope) and these will also be affected by the new setups. While, this may be important from a physical hydrology conceptualisation perspective (to maintain hydrological integrity), the results are not sensitive to changes in these parameter values.

For the Diep and Hoekraal River systems, K40A and K40B were divided into two and three sub-systems respectively. These subdivisions were based on the same reasoning as outlined for H10A-C in the previous paragraph. K40A_1 was designed to cover the higher topography represented by the land type Ib142, while K40A_2 represented the low lying area of the basin, marked by land types Gb2 and Db33. K40B_1 represented the higher topography (and land type Ib142), K40B_2 represented the middle level topography for this basin (land type Gb2) and K40B_3 represented the low lying, valley bottom topography (land types Db33, Fa39 and Ga3).

This approach to parameter estimation and model application managed to capture most of the variability in the parameters and reduced subjectivity in the interpretation of the basin physical data. The distributions of the parameters estimated for the subdivisions are given in Appendix C. The resultant simulations, using these parameters were improved over the simulations where parameter estimation was lumped within a given sub-basin. There was generally a substantial change in the ranges of variation (i.e. uncertainty) of the mean monthly flow (Q) and the mean gradient of the monthly FDC as presented in Figure 7.10 and Figure 7.11. Considered together with the effects of calibrating parameter GW, there is generally a progressive improvement in the model output ranges except for H10A in Figure 7.11 and Figure 7.14. The scale effects did not lead to an improvement in the range of variability of the slope of the FDC. There was also a shift of the FDC slope range from scenario D to A but with an overall increase in the range. It is concluded that scale significantly affects the model parameterisation and needs to be taken into account if predictive uncertainty is to be reduced. It is also likely that in ungauged basins the effects of scale can be overlooked given the absence of a control. Reducing the scale of modelling application therefore should improve the quality of predictions in ungauged basins.

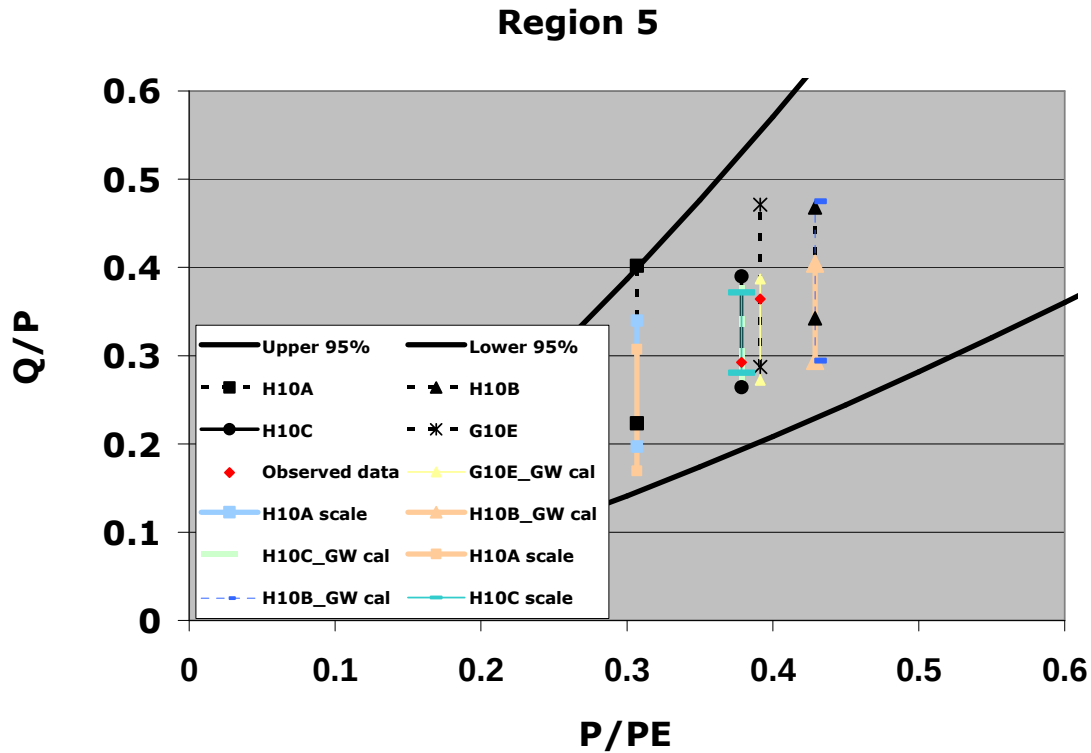


Figure 7.14 Changes in the ensemble Q/P ranges for the Region 5 as a result of the calibration of GW and the incorporation of scale effects.

7.5 Parameter sensitivity analysis of the ensembles

In the application of the constraints methodology, the idea is to assess behaviour of the model consequent on the variability in parameters, through indices of expected catchment functional behaviour. However, this behaviour is a sum of the effects of all the parameters and, as highlighted in Chapter 6, comparisons with the constraints tells us very little about the behaviour of individual parameters and the sensitivity of the model predictions to the individual parameters. In many cases it simply points to the basins where there are problems. It is therefore necessary to investigate and determine the effects of the individual parameters. In this study this is critical for the interrogation of the estimation equations and the determination of which parameters are important for which basins. This is invaluable for learning from the model, testing our understanding of process representations within the model and investigating both conceptual and structural consistency in the model. If conceptual expectations are at variance with the model outputs, it may be necessary to revisit both of them for a possible explanation. At times it is possible to increase parsimony in a model structure by simply assigning fixed values to the insensitive parameters. This

section outlines the results of this assessment. As pointed out in Chapter 6 both objective functions and flow metrics can be used to assess the parameter sensitivity. The objective functions are normally calculated from comparisons with observed data; however, in ungauged basins a time series representing conventional wisdom (e.g. WR90/2005 simulated flows) could also be used. An example of the summary of the sensitivity analysis based on all the different criteria available in this study is given in Table 7.4. The table shows the impact of different parameters on the different assessment criteria and gives insight into the most critical parameters and, therefore, the hydrologic processes likely to dominate in different sub-basins. Three arbitrary categories are defined for sensitivity defined by the degree of divergence of the normalised cumulative marginal probability curves of the parameters based on different assessment criteria. The categories range from highly sensitive, with the greatest divergence indicating the most sensitive parameter, through sensitive indicating moderate divergence, to insensitive with the least or no divergence. For instance, the parameter GW, as would be expected given the structure of the model, is a critical influence on the recharge flow metric and the objective functions which place an emphasis on the medium to low flows (i.e. TCE and TMMRE). It also seems that the parameters GW and FT are critical parameters for the sub-basins V70D and R20C, while POW and PI are critical for the sub-basin X31A and ZMIN and ZMAX are critical for C12D. One could therefore be persuaded to accept that subsurface runoff processes are important for the first two groups whereas surface processes are dominant in the last case. In a way, this is what one would naturally expect given that the first groups are wetter and more vegetated, while the latter is semi-arid. The analyses for the ungauged basins are based entirely on the constraints and similar conclusions can be made. In general the parameters are more identifiable when the cumulative frequency curves are distinctly separated from each other (e.g. Figure 7.15). If the frequency curves for the different groups cross each other the parameters are not identifiable.

Table 7.4 Summary of sensitivity analysis results for basins V70D, C12D and X31A. Black indicates a critical (highly sensitive) parameter, grey is important (sensitive) and white is negligible (insensitive).

Basin	Parameter	Flow metric			Objective function				
		MMQ	MMRch	FDC slope	CE	TCE	CE(Inv)	MMRE	TMMRE
V70D	PI1								
	PI2								
	ZMIN								
	ZMAX								
	ST								
	POW								
	FT								
	GW								
	T								
	S								
C12D	PI1								
	PI2								
	ZMIN								
	ZMAX								
	ST								
	POW								
	FT								
	GW								
	T								
	S								
X31A	PI1								
	PI2								
	ZMIN								
	ZMAX								
	ST								
	POW								
	FT								
	GW								
	T								
	S								
R20C	PI1								
	PI2								
	ZMIN								
	ZMAX								
	ST								
	POW								
	FT								
	GW								
	T								
	S								

Notes:

- MMQ refers to the mean monthly discharge
- MMRch refers to mean monthly recharge
- CE is the Nash Coefficient of Efficiency for the untransformed values, which TCE refers to the CE based on natural log transformed values. CE_Inv is the CE of the inverse values.
- MMRE is the % difference between the mean monthly flows of the untransformed simulated and observed data. TMMRE is the MMRE of the natural log transformed data.

7.5.1 Parameter sensitivity based on objective functions

For the gauged basins, it was possible to investigate parameter sensitivity based on any of the five objective functions (section 6.3). Figure 7.15 shows the results of the regional sensitivity analysis based on the Nash coefficient of efficiency (CE) objective function for the sub-basin of the Mooi River (T35C).

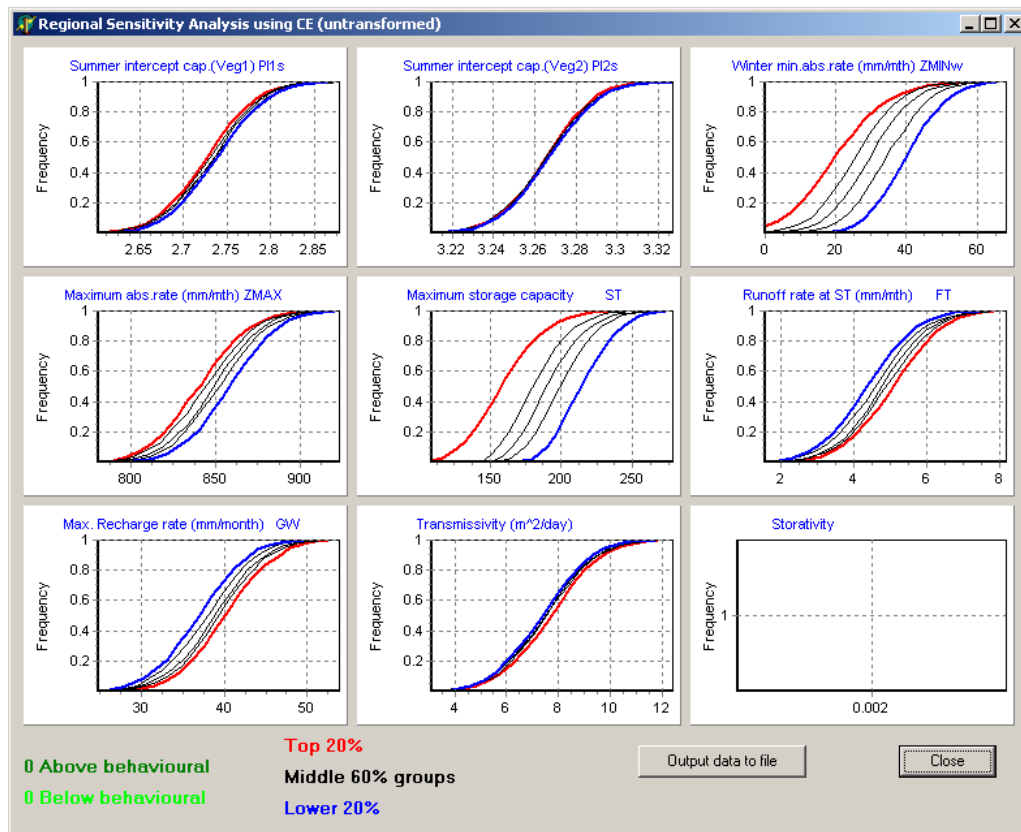


Figure 7.15 Parameter sensitivity analysis of the Mooi River sub-basin (T35C)

From the diagram it is easy to identify that the most critical parameters for this basin are ST and ZMIN. The highest divergence between the normalised cumulative frequency curves is for ST. From the diagram it can be observed that ZMIN, ZMAX and ST all tend to lower values for better CE values. However, the opposite is clearly true with parameters FT and GW which tend towards higher values for better CE values. Figure 7.4 confirms that the parameter estimation has resulted in somewhat lower than ideal values for these main runoff parameters. The sensitivity and identifiability of parameters may also be analysed and shown on scatter graphs. Figure 7.16 shows the scatter graph of the ST parameter for T35C and the trend towards lower values of the parameter for better CE values. The transmissivity (T) and PI parameters are not very sensitive.

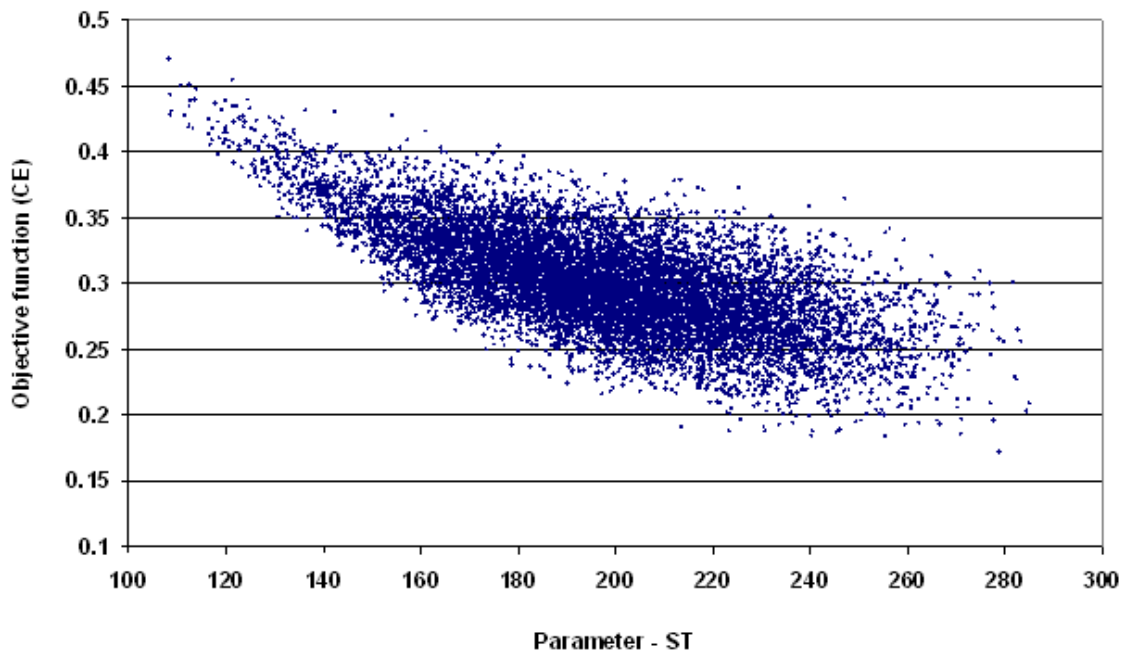


Figure 7.16 Scatter plot of the parameter ST for sub-basin T35C

Figure 7.17 is an illustration of the parameter sensitivity analysis based on the transformed CE (TCE) objective function for a sub-basin of the Berg River system (G10E) and shows that only parameters GW and T are sensitive with T tending towards higher values (above 12 m²/day), while GW tends towards lower values (below 20 mm), for improved TCE values. All the other parameters are insensitive.

Figure 7.18 illustrates sensitivity analysis based on MMRE for a sub-basin of the Gouritz River system (J33D). GW, FT and ST are the more sensitive parameters and for improved performance GW and FT require higher values (higher than about 15 mm/month in both cases), whereas ST tends to the lower values (about 100 mm).

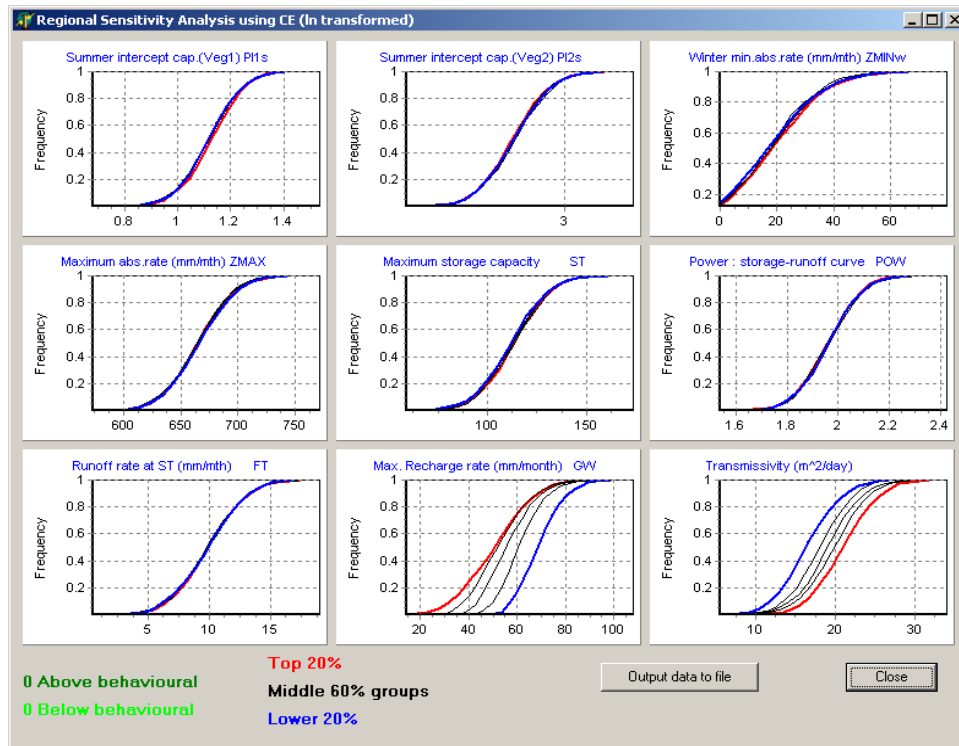


Figure 7.17 Sensitivity analysis based on TCE for a sub-basin of the Berg River system (G10E).

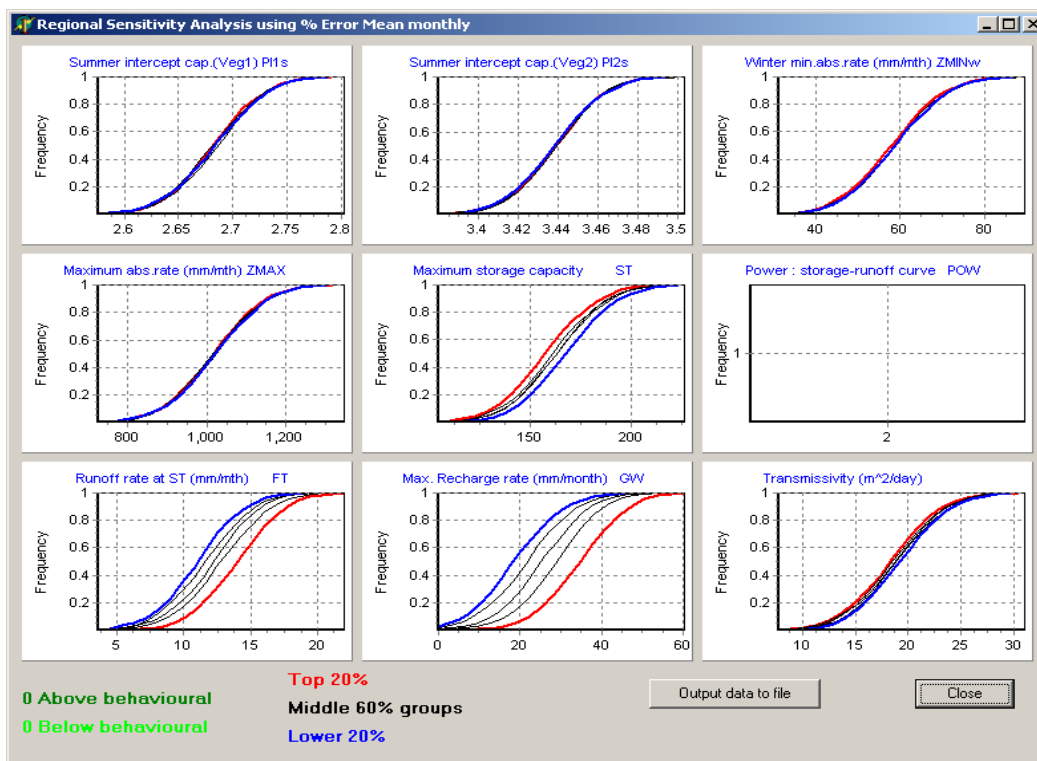


Figure 7.18 Sensitivity analysis based on MMRE for J33D, a sub-basin of the Gouritz River system.

7.5.2 Parameter sensitivity based on flow metrics

This sensitivity analysis works for both the gauged and the ungauged basins. Given the objectives of this study, this is especially important. Any of the five flow metrics calculated as an output part of .un1 text files can be used as an assessment criterion for parameter sensitivity. This assessment can also include an identification and quantification of the non-behavioural members of the outputs ensembles (i.e. the number of outputs above or below constraint limits). The sensitivity analysis complements the more detailed interpretation of the output data files, usually undertaken in a spreadsheet program. If most of the outputs are rejected as non-behavioural, that suggests the existence of a problem that warrants investigation in the same manner as discussed in section 7.3. Figure 7.19 and Figure 7.20 illustrate regional sensitivity analyses for K40B (a sub-basin of the Hoekraal River system) and R20B (a sub-basin of the Buffalo River system) respectively.

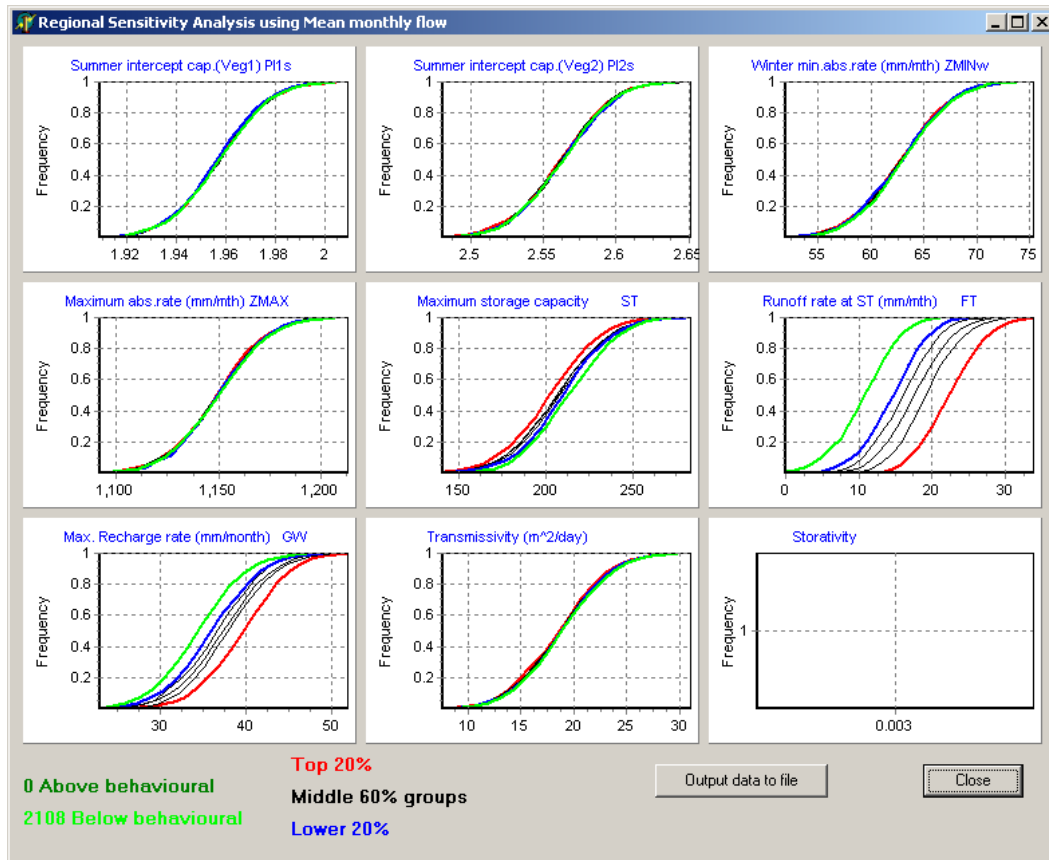


Figure 7.19 Regional sensitivity analysis of the mean monthly flow metric for K40B before the GW parameter was calibrated. After the calibration all non-behavioural outputs were eliminated.

While both have non-behavioural outputs, there are more for K40B (2108 out of 10 000), all of which are below the lower limit of the constraint (scenario D), whereas R20B has fewer (878 outputs) all above the upper constraint limit (scenario A). The sources of these uncertainties are also different. In K40B, parameter FT accounts for the bulk of this uncertainty. GW accounts for some of this uncertainty, with all the other parameters being relatively insignificant. Despite the apparent importance of FT, after calibration of the GW parameter against GRAII recharge constraints all the non-behavioural results were removed. This illustrates the interrelationships between the two parameters that dominate the low flow regime (GW and FT). In R20B, the non-behavioural outputs are a result of the variability in parameter ZMAX, with only ZMIN, amongst all the other parameters, making some minor contribution.

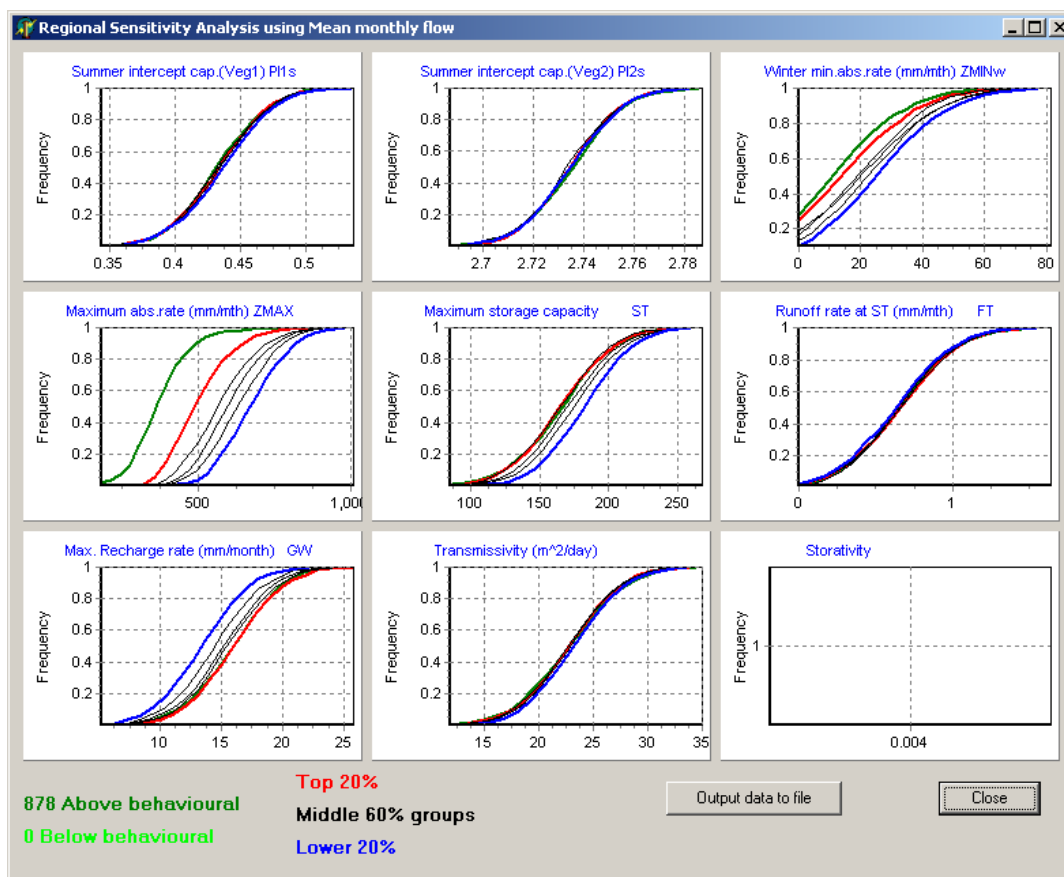


Figure 7.20 Regional sensitivity analysis of the mean monthly flow metric for R20B.

Figure 7.21 shows the results of regional sensitivity analyses of the constraints for the basin V70D. The parameters FT, ST, ZMIN and GW are the most sensitive based on the mean monthly flow signature, which is no surprise given an understanding of the structure of the model. There are a small number of non-behavioural ensembles (68), all of which are above the constraint. These are not caused by any single parameter, but by combinations of low values of ZMIN, ST and POW, possibly combined with high values of FT and GW. This represents a typical result for a sub-humid catchment where non-behavioural ensembles are caused by inappropriate parameter combinations rather than inappropriate values for single parameters.

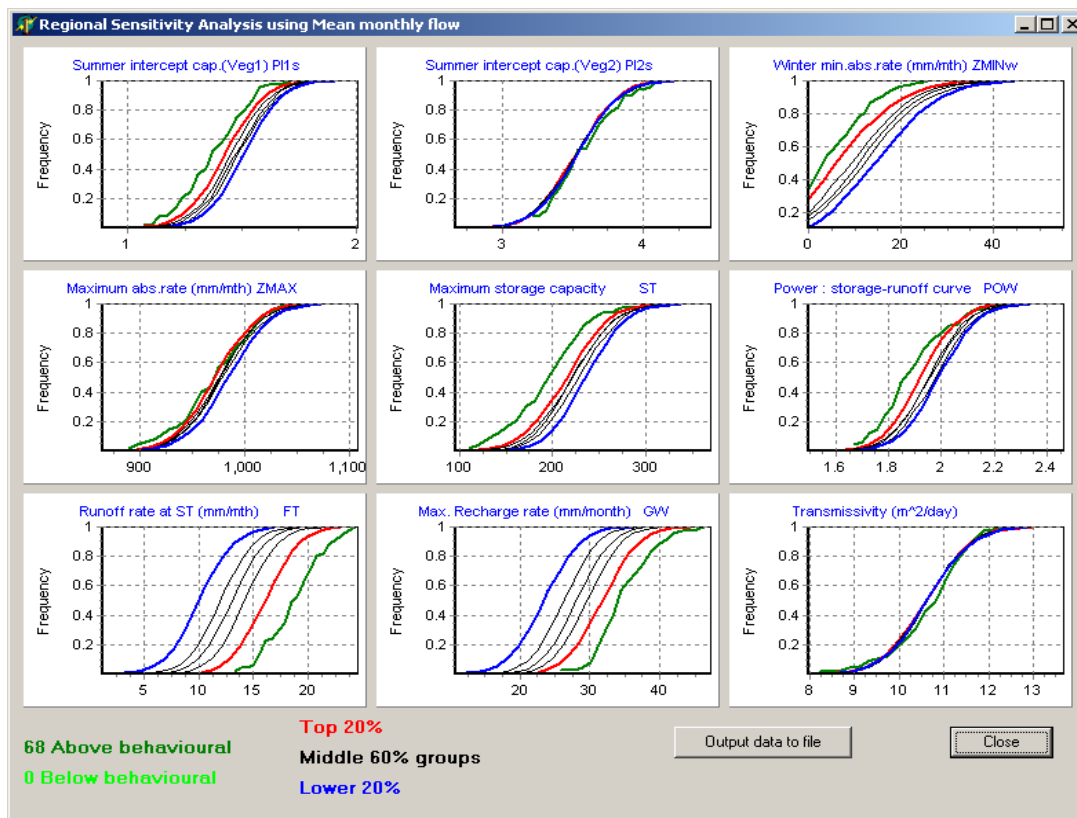


Figure 7.21 Regional sensitivity analysis of the mean monthly flow for the Little Boesmans River sub-basin (V70D)

For purposes of illustrating the effect of different metrics, the same sub-basin was used. The analysis based on the recharge constraint confirmed the dominance of the parameter GW (Figure 7.22) and that there is a very clear distinction between the results for low parameter values versus high values. This suggests that the recharge constraint can be very useful in that it addresses uncertainty in only one component of the model, unlike the mean monthly flow constraint. However, its usefulness depends upon having good regional constraint data but unfortunately the information from the GRAII database contains too much uncertainty at present.

Figure 7.23 illustrates that the simulated slope of the FDC in the V70D basin is strongly influenced by the low flows generated from ground water recharge and subsequent discharge. Most of this influence is related to parameter GW (as might be expected), but ST and ZMIN are also influencing the results.

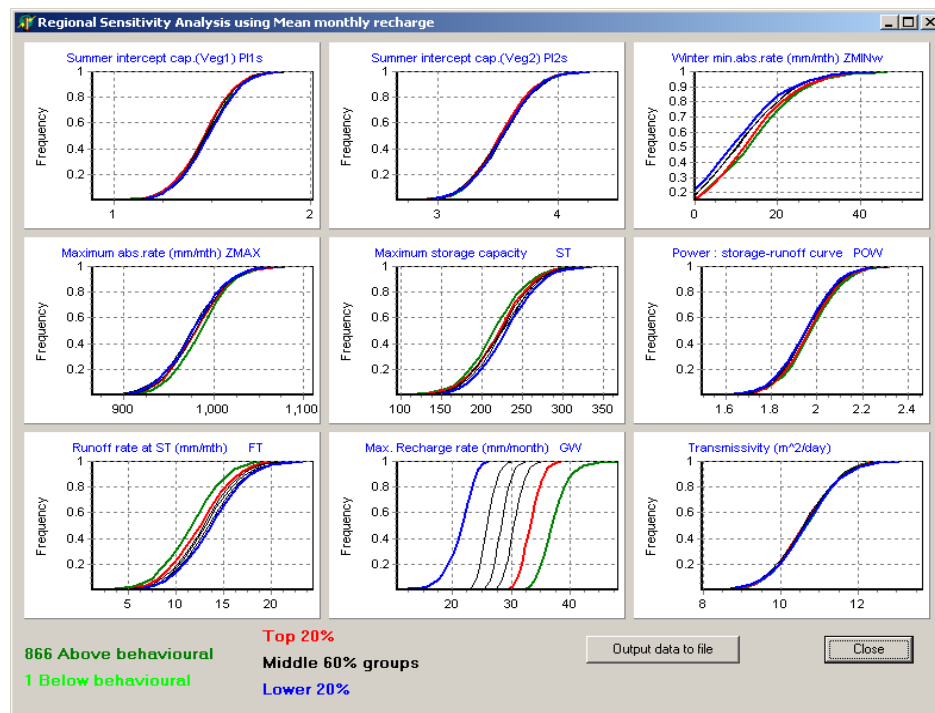


Figure 7.22 Regional sensitivity analysis of the mean monthly recharge for the Little Boesmans River sub-basin (V70D)

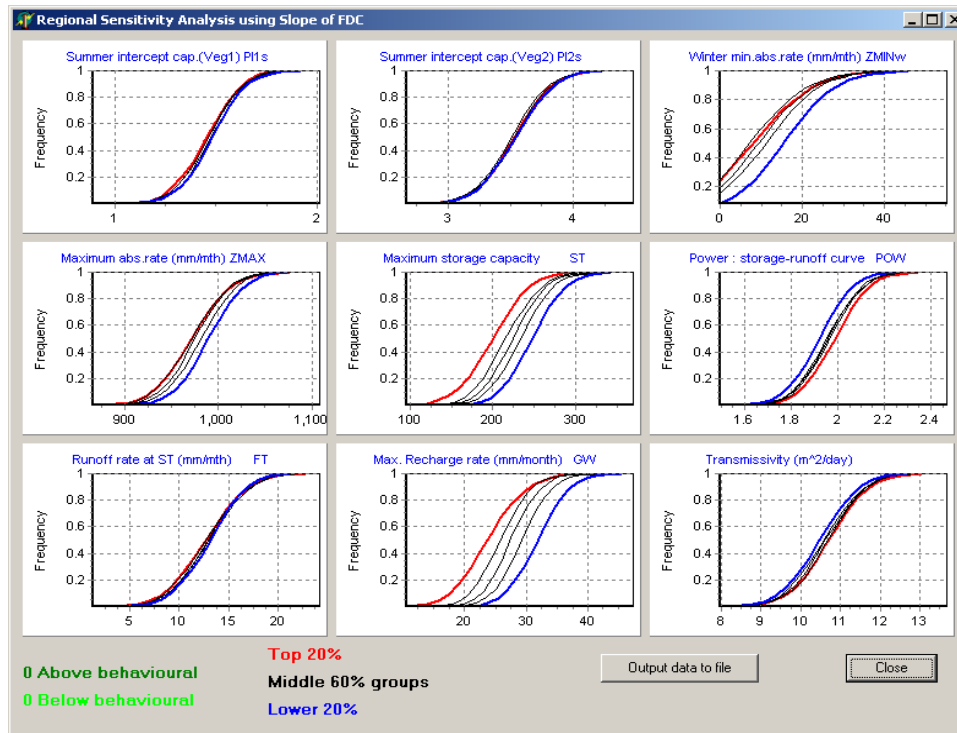


Figure 7.23 Regional sensitivity analysis of the slope of the monthly FDC for the Little Boesmans River sub-basin V70D.

It should be noted that while it is possible to interpret the sensitivity results based on objective functions for trends in parameters that give improved objective function values, the same cannot be done with flow metrics. The flow metrics can indicate which are the most identifiable parameters and do not provide any other information about which parameter sets give better results.

7.6 Concluding remarks

The proceeding results show that there is a lot of potential for the use of the uncertainty framework for South African basins. In a typically ungauged basin, the constraints can be used as a surrogate for observed data to 'calibrate' the model. The three constraints used in this study are robust enough to cover the range of geo-physical and hydro-climatic conditions in South Africa. It is also logical to assume that the same approach can be used (with minimum modification to account for differences in data availability and quality) in other basins within the southern Africa region. The incorporation of uncertainty into the regional application of the Pitman model has been achieved with generally acceptable results, although there is room for improvement. The following concluding remarks can be drawn from the results in this chapter:

- ❖ The use of constraints can significantly condition predictions in both gauged and ungauged basins of South Africa. While this is so, it is unknown how the constraints developed for other basins outside South Africa will fare given the differences in data availability and quality. However, the use of hydrological constraints is a viable option in hydrological predictions and should be encouraged.
- ❖ Constraints are an important surrogate for observed historical data and can be used for 'calibrating' models especially in ungauged basins. However, there are situations when all the outputs are behavioural but the ensemble ranges are too large. This may be a problem for model-based decision making. This implies that either the limits of acceptability based on the constraints would have to be reduced or that additional constraints need to be developed. It is not clear at this stage of the development of the framework which option is likely to be achievable given the available data.
- ❖ There are two questions that are related to the previous point. Firstly, how many constraints are necessary or are needed? This is not easy to answer and to a large extent depends on the quantity and quality of data available to develop the constraints. It is prudent to note that it is pointless to

develop constraints that assess the same component/aspect of hydrology, a classic case of redundancy that usually occurs among scientists in the selection of hydrologic indices (Olden and Poff, 2003). It would be sensible to investigate and constrain as many components of the simulated flow regime as possible in the manner of multi-criteria calibration suggested by Boyle et al. (2003). The second, relatively easier, question pertains to the application of these constraints. What is the order of application of the developed constraints? This is important when more constraints are being used and it is possible to reject all outputs based on one constraint but accept them based on a different one. Also, the order of application may differ between and among users which may potentially lead to different results. There should therefore be a structured way of applying constraints so that consistent results can be obtained. It is also possible that the constraints to be used could depend on the type of basin under investigation as not all constraints would be useful.

- ❖ While the constraints have worked fairly well, the ground water recharge constraint is not currently based on good enough data. It would be better to design the constraint based on a single method of determination of the control recharge values for consistency.
- ❖ While most of the parameter estimation routines appear to have worked successfully to give reasonable uncertainty distributions, it is obvious that the routine for the ground water recharge parameter needs to be revisited in order to produce better estimates in all basins and avoid resorting to calibration.
- ❖ The interpretation of the basins physical characteristics data and the scale of model application and parameter estimation have been highlighted as having significant impacts on the level of uncertainty in the model outputs. However, there were a large number for which the use of a reduced scale did not improve simulations. It is therefore concluded that the appropriate scale of application should be decided from a consideration of the variability of the physical properties within any specific basin.

The use of the constraints for guiding model application in both gauged and ungauged basins has advantages for use in regions such as southern Africa where data for model calibration are scarce. However, there is need to establish the level of uncertainty related to the constraints themselves for purposes of quality control of the resulting acceptable behavioral outputs.

Some parameter equations and the approach to defining uncertainty bounds need to be revisited. The constraint diagrams and the regional sensitivity can be used to effectively identify areas where improvements are required (Figures 3.5 and 6.10). Such feedback is essential for the further development of the parameter estimation procedures and the application of the framework. Currently, some of the constraints exhibit wide ranges that may be too large and result in ensemble ranges that are too large for effective use in system yield models. Such a large amount of uncertainty is expected to result in resource availability estimations that are too uncertain for effective decision making. Therefore, it is imperative that these ranges be narrowed and contribute to less uncertainty (and therefore risk) involved in basing decisions on model outputs.

CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

8.1 Introduction

This chapter aims to synthesize the main findings of this study, relate them to the stated aims and objectives, and outline some recommendations for further work. Water resources planning and management have for a long time been based on data generated by models, even in poorly gauged basins, and mathematical models have become a critical part of decision and/or policy making as hydrological systems have been increasingly affected by human demands. Contemporary applications of models in ungauged basins have been based on any one of the many techniques of regionalization. The Pitman model has enjoyed relatively widespread use in southern Africa, and for South Africa, regionalized model parameters have been developed based on mapping using somewhat subjective measures of similarity between and among basins. In the rest of the southern Africa region there are no regionalized parameter values available, but the same similarity techniques have been generally applied for ungauged basins. While the results have provided a basis for decision and/or policy making, it is generally acknowledged that they are not without uncertainty and rely to a large extent on model user experience. The uncertainty is a result of a number of issues including a high degree of temporal and spatial variability of hydro-climatic conditions, input data scarcity, parameter estimation methods, model structural inadequacies and poorly defined water use data and land use changes. In spite of this recognition of the existence of uncertainty there has been little effort to explicitly account for the uncertainties involved (Sawunyama, 2009). The dominance of model parameter uncertainty in the Pitman (Pitman, 1973) model is a result of the large number of parameter to be estimated, and the inability of typically used objective functions to determine these parameters. A model with fewer parameters would tend to have small uncertainty (greater precision) but generally at the cost of a reduction in representation of the catchment behaviour (reduction in accuracy).

The PUB initiative has led to an increase in the awareness of the impacts of uncertainty on the predictions of hydrological variables and, more importantly, the need to directly account for and incorporate uncertainty into decision support tools. In considering uncertainty, three issues have to be addressed for any

improvement in water resources decision making and these are understanding, quantification and reduction of uncertainty. While the literature contains various approaches to the uncertainty problem, few address the last aspect in any detail (Ajami et al., 2007). From a practical point of view, there is little point addressing the issues surrounding uncertainty if there is no effort to reduce it. In a management context it is important that unambiguous guidance be provided when model results are uncertain. Of practical relevance to South Africa and southern Africa is the applicability of the myriad of approaches to uncertainty. Given the types of models used (and the conventional knowledge based on these models), the scarcity of historical observed data and the modelling culture of practitioners within the region, it is imperative that a common understanding and approach be developed for achieving the multiple water resources objectives of the region. Of the three major sources of uncertainty in hydrological modelling, this study has focused on parameter uncertainty. The main reason is that parameter uncertainty appears to contribute the most to predictive uncertainty in the outputs of the Pitman model as applied in southern Africa (Sawunyama, 2009). The development of the uncertainty methods has been undertaken within the context of a model independent uncertainty framework that will eventually accommodate other sources of uncertainty.

8.2 An uncertainty framework for model application

This study represents a contribution towards the explicit incorporation of uncertainty in making hydrological predictions. A framework for the incorporation and estimation of uncertainty is suggested and tested for basins in South Africa. The main components of the framework relate to the estimation of parameters (section 8.3) and their probability distributions (section 8.5), indices of catchment functional behaviour (constraints, section 8.6), sensitivity analysis (section 8.7) and provision for a feedback loop. The estimated parameter priors are used to generate ensembles of model simulations which are then assessed using regionalized constraints. It is implicit in the framework that the constraints are based on the best available knowledge covering different regions. The components of the framework are considered robust enough to enable its use with any model structure. One of the main findings of this study is that the application of the framework with the Pitman model has demonstrated its merits. The framework is capable of being used in both gauged and ungauged basins. However, its successful use outside South Africa will depend on data availability and quality. This will necessitate some adjustments to the components to adapt

to these different conditions. It should be noted that the development of a framework was not a primary objective of the study, but emerged out of the development of the parameter estimation process. Due to the wide variation of data within South Africa and across the region it became apparent that there was a need for a consistent approach and this is achieved through the proposed framework.

8.3 Parameter estimation procedures

Most contemporary model applications in both gauged and ungauged basins have relied on the adjustment of parameters to match the simulated hydrograph to that of the uncertain observed record. For instance, there are uncertainties related to the extent to which the available observed flows represent the natural hydrology of the basins. Human influences on most rivers within the southern Africa region, in the form of small scale river (and off-river) storages (farm dams), return flows and run-of-river abstractions, are inadequately quantified. In this study the parameters of the Pitman model have been directly quantified from measurable basin physical attributes. Well known physical hydrology principles are used to infer relationships between the conceptual model parameters and the basin properties. This parameter estimation approach has managed to produce hydrologically relevant parameters that have resulted in largely acceptable results across the hydro-climatic and geo-physical conditions examined in this study. The parameters that were estimated in this study relate to all the natural processes simulated by the model and the *a priori* estimation approach has been successful and is robust. The relationships between the parameters and basin descriptors have adequately accounted for the variability in the basin property data. This has maintained the physical integrity of both the model and parameters. The standard estimation procedures give the mean value ('best' estimate) of a parameter based on the physical characteristics of the basin. The results of this study suggest that the model and the parameters are capable of adequately representing the basin natural hydrological processes. The model is adequately parameterized and those parameters do not represent the effects of multiple processes. However, the interactions between and among the parameters often make it difficult for the parameters to be identifiable (see section 8.7). The estimation procedure for the parameter GW has not worked quite as well as the others in some basins. There is no apparent hydro-climatic or physical bias in this failure and therefore there are no clear indications of how the estimation approach could be improved.

8.4 Basin physical property data for parameter estimation

The success of application of the methods described here will depend to a large extent on the availability and quality of data to quantify the hydro-meteorological and geo-physical attributes of the catchment. The development of the estimation equations has been premised on the availability of data that are collected by many different departments within the region and these include soil hydraulic properties, soil texture type and depth, basin slope, relief, vegetation cover and geology. The availability of these data across the region is variable, neither are they easily accessible nor of the same level of detail nor quality. This was expected given the diversity of the region. The data available for South Africa is the most detailed (covers many of the required basin attributes), has the best spatial coverage (available at the national scale) and are of better quality (i.e. reasonably quantified basin attributes) compared to the other parts of the region. Notwithstanding some problems of detail in some places, the AGIS (2007) database available in South Africa has provided a reasonably solid foundation for development and testing of the parameter and uncertainty estimations. The ultimate goal is to transfer these estimations to other places in the region after learning from the South African experience. There will be need to assess the degree of variability in the basin property data with the intention of providing guidelines for the use of the methods to basins outside South Africa. In many cases the estimation process will not be easy and will involve subjective interpretation of hugely qualitative information (Kapangaziwiri, 2008), which will make the incorporation of uncertainty through the use of ranges of variability (see section 8.5) a big challenge.

The implication is therefore that in places outside South Africa a standard will be needed to define appropriate mean values and/or limits or ranges for the qualitative data in order to increase objectivity and consistency. For instance, it is necessary for the estimation processes that attributes such as soil depth and slope angle have quantitative mean values or boundaries around such descriptions as 'deep soil' or 'steep slope' so that they mean the same throughout the region. The current situation outside South Africa implies that the uncertainty related to the nominal qualitative basin information will be very large, and the need to reduce it implies that more and better quality data would need to be collected. However, it was observed in this study that even data of relatively high resolution can also be in error. For instance, in the case of K40B in South Africa, the application of the model at a finer scale did not reduce the uncertainty. This is

thought to be associated with extrapolation from a limited sample of field data used to construct the land types. Personal knowledge of the area suggests a larger variability than is represented in the AGIS land type data. While there is no evidence available for similar problems in other parts of South Africa, it is not unreasonable to assume that they exist, given that only limited field observations were used.

8.5 Incorporating uncertainty into parameter estimation methods

The standard parameter estimation equations provide a single value for a given parameter in any chosen basin. Given the variability in the basin physical attributes data, this approach is not very informative and is quite uncertain. A simple example is that two basins may have the same (mean) value of 15% for, say, basin slope but with different variability characteristics. If basin A has a slope range of 13 to 18 and basin B has range 5 to 45, these basins will essentially be different in the way they impact the estimation process if their variabilities are taken into account. The estimated basin slope for A is far less uncertain than that for B. The uncertainty framework was therefore developed to be a consistent platform for the incorporation of uncertainty into the estimation process. To account for the uncertainty in the parameter estimation process, the ranges of variability of the basin attributes data were used to represent their frequency distribution characteristics. While many distributions are possible for natural phenomena (Munoz-Carpena et al., 2007), the distributions used in this study were based on the premise that some values are more likely to occur than others for both the physical basin property data and the parameters. Thus, Normal distributions (defined by a mean value and standard deviation) were used for the physical basin attributes and this appears to have worked well in all basins and has been justified by the results. The uncertainty estimation procedures allow the use of the Uniform distribution where information on the physical basin attributes is inadequate or where no estimation equation exists for a given parameter. However, this requires that appropriate boundary values be set to define the feasible parameter space. Simulation results based on the normally (or log-Normal in cases of large skewness in secondary inputs and/or resultant parameters due mainly to estimation of largely non-linear process) have been largely within expected ranges. In general, the model output ensembles generated by the parameter distributions have reasonable ranges of uncertainty but further work is required to ensure greater consistency in the results. In cases

where the parameter distributions resulted in ensemble ranges that were quite large, many had appropriate (behavioural) mean values. This suggests that the focus of future work should be on the standard deviation estimates of the parameter distributions.

8.6 Use of constraints in assessing output uncertainty

Three indices of hydrological response behaviour were developed and tested as constraints, and the study showed that the regions and the regional relationships established were hydrologically sensible and in general agreement with existing knowledge. The use of the constraints to condition model simulations provides a multi-criteria calibration and the tests of the current group in this regard suggests that more indices may need to be developed to constrain more components of simulated flow. The preliminary set of constraints developed for this study relate to the overall water balance component (volume constraint, runoff ratio), the variability of the flow regime (slope of the FDC) and ground water recharge. It should be noted however that the development of constraints is heavily reliant on the availability and quality of data. In this study, simulated flows had to be used in the initial development of some of the constraints due to the inadequacy of the observed data. However, the use of these data (affected by modelling artefacts) did not adversely affect the constraints. They were used for the initial development of the constraints before observed data were used to finalise the relationships. Therefore, constraints are also subject to uncertainty and in this study uncertainty bands were developed around the regional constraint relationships. These bands therefore determined the limits of acceptability when the model output ensembles were compared with the constraints. The basis of this approach was that the uncertainty related to the constraints was initially assumed to be less than that related to the parameters. In that case the constraints can therefore be used to reduce predictive uncertainty. Comparing the model output ensembles with the regionalized constraint relationships gives four possible categories of uncertainty, ranging from low uncertainty, through bias towards either the low or high flows to large uncertainty. The constraints have worked well in many of the basins and the results are encouraging. However, the groundwater recharge constraint may need revisiting at a later date. This constraint is based on data from three different methods whose uncertainties have not been determined. It would be more logical to base the constraint of a data set based on one method only. Notwithstanding this, the groundwater recharge constraint resulted in many behavioural outputs with low levels of

uncertainty. What is difficult to determine at the moment is the extent to which this is a result of the large boundaries determined by the data used. The FDC slope has been applied at the national scale as a result of difficulties in regionalizing the constraint. This has resulted in wide bands for the constraint, which was expected given the wide variability of hydro-climatic and geo-physical conditions within the country. The model ensembles generally resulted in FDC slopes that were biased toward the lower boundary of the constraint range.

One of the issues that arise with the application of a number of constraints is the need for an application procedure that clearly outlines the order of application of the constraints, i.e. which constraint is applied first. In this case, the fact that the use of the groundwater constraint necessitates re-calibration makes this consideration important. However, in the absence of such problems the definition of an order of application of the constraints is not required. In fact, it is possible and even desirable to handle the constraints simultaneously as in multi-criteria (or Pareto optimization) analysis. The other issue relates to the number of constraints necessary for a region like southern Africa. While it is sensible to develop as many constraints as possible, it is also prudent to guard against redundancy where constraints examine the same components. It was demonstrated in this study that constraints can be used effectively to guide model application where historical observed flows are not available.

8.7 Sensitivity analysis and the feedback loop

An important aspect of the framework is the inclusion of a sensitivity analysis that can be used to gauge the impact of individual parameters on the simulated flow. The use of the sensitivity analysis enables an examination of the identifiability of the parameters. In the Pitman model, the identifiability of parameters is usually a problem due to the number of parameters and the interactions between them. This analysis managed to show the differences in the process dominance of the different basins. The semi-arid, surface runoff dominated sub-basins (e.g. C12D, D55C and A42D) showed that the infiltration parameters (ZMIN and ZMAX) were critical, while for the baseflow driven catchments (e.g. X31A, V70D and V20A) the critical parameters were generally FT and GW. Generally, the results were consistent with expectations from an understanding of the physical hydrology of the basins tested. The results of this study support the suggestion that the identifiability of a parameter is related to its importance in representing the basin's response (McIntyre et al., 2005).

The sensitivity analysis is a vital step of the feedback loop of the uncertainty framework. While the constraints identify the basins where the application of the parameter estimation process has failed to work properly, this is not informative enough for the estimation process if remedial action is to be taken. Sensitivity analysis identifies the parameters with the greatest variability and that influence the model results the most. This then informs the reassessment of the estimation approach for these parameters. Such problems related to the scale of model application, degree of variability, and interpretation, of the basin physical properties information are clearer to deal with when the parameters that are most affected can be identified.

8.8 Recommendations and general remarks

Based on the outcomes of this study, the following recommendations are suggested:

- ❖ While the framework for incorporating uncertainty designed for southern African conditions has shown great potential, there exists scope to further refine some of the regional relationships, and the recommendation is to build on this framework. In spite of the fact that some of the components of the framework are not perfect, its use is expected to contribute to more consistent results and provide a basis for comparison of results from different models and different model users. It also provides an approach for regional application of models in ungauged basins.
- ❖ Uncertainty estimation should become an integral part of water resources management within the region.
- ❖ Despite the fact that the calibration of the GW parameter based on the GRAII data seems to have provided a solution to the simulation of the recharge component of the model, it is still necessary to develop a better estimation equation.
- ❖ More constraints need to be explored in order to constrain as many components of simulated flow as possible. Where insufficient data exist, as is likely to be the case in some places within the region, the same constraints can be used but with larger uncertainty, represented by wide bands.
- ❖ The optimization of the model outputs based on the constraints (i.e. a multi-objective assessment using the constraints as objective functions) should be investigated for use in ungauged basins. This could contribute to the optimization of parameter sets that are within the behavioural output

space. Instead of generating a single optimum solution, an optimum ensemble of model outputs.

- ❖ The methods need to be tested in some basins outside South Africa to provide a clearer idea of the issues involved and the expected problems and how they can be solved.
- ❖ While the uncertainty analysis for adequately gauged basins is straightforward, the possible conjunctive use of short or incomplete records and highly uncertain constraints needs to be explored in the future. As this study draws to an end, it is becoming clear that in some parts of the region all the available information should be used to improve water resources management.
- ❖ While the subjectivity in the estimation process can be reduced by applying the model at a finer resolution, this approach may be difficult outside South Africa. It is therefore necessary to investigate how uncertainty would be reduced in such situations. One way is to increase the collection of more and better quality data.
- ❖ Explore the use of other sources of information to develop estimation of both the parameters and the constraints.

As the demand for water resources of southern Africa increases (in terms of both the quantity and quality) there is need to adequately take stock of the available resources. While it may be impossible to be absolutely certain about the stocks available, quantifying the uncertainties related to the estimation process would increase confidence in the scientific determination of stocks. Most of this determination is based on model simulations but the accuracy of the results is unknown. Uncertainty analysis should allow us to express our confidence in the model results. Failure to account for the estimation uncertainties could lead to unjustified confidence in hydrological and water resource estimations and predictions. It could also lead to a lack of appreciation of the risks associated with decision making in uncertain situations, and suppresses the incentive to improve data collection frequency and techniques, parameter estimation methods and model structures. The inclusion of uncertainty in water resources estimation tools, however, entails rethinking the way models are applied and how results should be interpreted and communicated to stakeholders. The framework discussed in this study is an attempt to achieve consistency in the way uncertainty can be incorporated and analysed within water resources estimation tools.

This study concentrated on the incorporation and analysis of parameter uncertainty into the Pitman model through a model independent framework. It is acknowledged that many other sources of uncertainty may impact on predictions in ungauged basins, but this framework allows for the incorporation of these in the future. It is not enough to only design elegant frameworks and tools but to be able to effectively communicate the results of these methods to stakeholders such that informed decisions can be made. Incorporating uncertainty in hydrological models improves the ability of the modelling community to meet the requirements for decision making by providing a sufficiently broad spectrum of possibilities that enable the assessment, quantification and incorporation of risk into the policy and/or decision making process. The dictum to be followed here is that the reliability of the decisions would increase if the uncertainty bands are wide enough to be credible but narrow enough to be useful. Uncertainty should increase the confidence in model predictions of future change rather than relying on a model that has only been shown to reproduce historical conditions at the site of interest. In the context of South Africa, the incorporation of uncertainty into the generation of natural hydrology should be followed by a discussion on how these results can be used further in water resources systems models to generate uncertain present day and future scenarios. It is intended that the use of the framework will galvanise the collection of more relevant data and use of other data sources such as remote sensing. However, Hughes and Kapangaziwiri (2009) contend that there are still some pertinent scientific questions to be answered such as “how much of the uncertainty that we are modelling is real uncertainty or do we know more about hydrological responses at ungauged sites than the current results suggest?”

Finally, it seems that there is still some uncertainty about uncertainty.

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APPENDICES

Appendix A. Physical descriptions of the test basins used in this study.

Sub-basin	Gauge	Physical description
A42A	Ungauged	Undulating to steep topography, moderate to deep sandy loams; fractured sedimentary strata.
A42B	Ungauged	
A42C	Ungauged	
A42D	A4H008	
A42E	Ungauged	
A42F	Ungauged	
A92A	A9H004	Undulating topography, moderate to deep sandy loams; sedimentary rocks with intrusive dykes and sills
B41G	B4H009	Undulating to steep topography, moderate to deep sandy loams; ultra metamorphics
C12D	C2H004	Undulating topography, moderate to deep clayey soils, inter-bedded shales and sandstones
D55C	Ungauged	Undulating topography, shallow sandy loams; inter-bedded mudstones, shales and sandstones.
G10E	G1H008	Steep topography, moderately deep, porous sandy loams with some impermeable lenses; unconsolidated sedimentary strata.
H10A	Ungauged	Steep, moderately deep sandy loams; Karoo shales and sandstones.
H10B	Ungauged	
H10C	H1H003	
J33C	Ungauged	steep topography, shallow sandy loams; fractured mudstones, shales and sandstones
J33D	Ungauged	
K40A	K4H003	Steep topography, shallow to moderate loamy sands; fractured granite. Present day impacts of plantations.
K40B	K4H001	
M10B	Ungauged	Steep topography, shallow, sandy loams; inter-bedded mudstones, shales and sandstones.
N24A	Ungauged	Undulating topography, moderate to deep, sandy loams; inter-bedded mudstones, shales and sandstones.
Q14A	Ungauged	Undulating topography, moderate to deep, sandy loams; inter-bedded mudstones, shales and sandstones.
Q92F	Ungauged	Undulating topography, moderate to deep, sandy loams; inter-bedded mudstones, shales and sandstones.
R20A	Ungauged	Undulating topography, moderate to deep sandy loams; inter-bedded mudstones, shales and sandstones.
R20B	Ungauged	
R20C	R2H006	
R20D	ungauged	
S60C	S6H003	Undulating topography, moderate to deep, sandy loams; fractured granites.
T35C	T3H009	Steep topography, moderate to deep, clayey loams; fractured granites.
T40A	Ungauged	Undulating topography, moderate to deep sandy loams; fractured sedimentary strata.
T40B	Ungauged	
T40C	T4H001	

Sub-basin	Gauge	Physical description
U20A	Ungauged	Undulating topography, moderate to deep clays; fractured sedimentary strata.
U20B	U2H007	
U20C	Ungauged	
V20A	V2H005	Undulating to steep topography, moderate to deep clayey loams; Karoo shales, sandstones, grit and coal.
V60A	V6H006	Undulating topography, moderate to deep clay to clay loams; mainly inter-bedded mudstones, shales and sandstones with fractured sedimentary strata.
V60B	V6H004	
V70D	V7H012	Steep topography, moderate to deep, clayey soils; inter-bedded mudstones, shales and sandstones.
X11A	Ungauged	Undulating topography, moderate to deep sandy clay loams; inter-bedded mudstones, shales and sandstones.
X11B	Ungauged	
X11C	Ungauged	
X21A	Ungauged	Undulating to steep topography, moderate to deep sandy clay loams; porous sedimentary strata.
X21B	Ungauged	
X21C	Ungauged	
X31A	X3H001	Steep topography, moderately deep sandy clay loams; dolomites and limestone.

Appendix B: Parameter distributions (mean μ and standard deviation σ) for some basins before and after GW calibration. GW1 and GW2 refer to the parameter distribution before and after calibration respectively.

Basins	A92A		C12D		G10E	
parameters	μ	σ	μ	σ	μ	σ
PI1	2.132	0.000	0.480	0.034	1.155	0.106
PI2	2.873	0.017	2.964	0.018	2.760	0.017
ZMIN	44.250	22.012	15.095	1.467	48.750	23.488
ZAVE	194.197	0.000	256.936	0.000	169.374	0.000
ZMAX	926.200	35.697	671.800	38.043	1131.400	57.367
ST	211.692	27.058	134.265	21.299	118.835	15.188
POW	1.990	0.040	2.900	0.550	2.000	0.000
FT	9.825	3.571	0.637	0.123	10.737	2.577
GW1	55.932	4.593	34.697	10.368	61.530	12.560
GW2	60.000	3.500	23.000	5.500	15.000	2.500
T	4.000	0.800	40.000	8.000	20.000	4.000
S	0.005	0.001	0.005	0.001	0.003	0.000

Basins	H10A		H10B		H10C	
parameters	μ	σ	μ	σ	μ	σ
PI1	0.348	0.022	0.357	0.022	0.601	0.067
PI2	2.796	0.017	2.882	0.018	2.348	0.013
ZMIN	65.000	0.000	80.000	0.000	93.600	7.110
ZAVE	269.384	0.000	247.970	0.000	774.178	0.000
ZMAX	1132.000	31.398	1199.800	2.000	999.600	38.136
ST	160.743	16.129	182.565	16.674	166.492	23.261
POW	2.000	0.000	2.000	0.000	1.930	0.100
FT	19.895	3.896	19.068	3.802	36.554	17.428
GW1	35.394	9.195	59.547	6.995	29.112	5.175
GW2	13.500	2.250	22.500	2.250	15.000	2.000
T	42.400	4.240	40.000	4.000	50.000	10.000
S	0.001	0.001	0.001	0.001	0.001	0.001

Basins	M10B		V20A		X21A	
parameters	μ	σ	μ	σ	μ	σ
PI1	1.003	0.093	1.296	0.113	0.739	0.033
PI2	2.388	0.015	3.099	0.019	3.189	0.019
ZMIN	45.000	0.000	55.550	17.479	22.974	1.318
ZAVE	83.750	0.000	1143.060	0.000	338.742	0.000
ZMAX	820.000	0.000	1200.000	0.000	593.600	50.282
ST	115.765	9.435	276.565	41.145	168.266	28.558
POW	1.970	0.070	2.000	0.000	2.650	0.220
FT	10.234	3.200	102.341	23.013	0.654	0.271
GW1	41.193	11.926	59.477	6.929	42.327	6.284
GW2	17.500	3.750	48.500	3.250	30.500	4.250
T	20.000	4.000	120.000	20.000	11.840	4.000
S	0.001	0.000	0.004	0.000	0.001	0.001

Basins	R20A		R20B		R20C		R20D	
parameters	μ	σ	μ	σ	μ	σ	μ	σ
PI1	2.030	0.017	0.445	0.031	1.308	0.116	0.474	0.034
PI2	2.752	0.016	2.740	0.017	3.105	0.019	2.919	0.018
ZMIN	56.700	28.676	22.950	20.623	23.850	11.846	25.950	24.034
ZAVE	388.736	0.000	322.059	0.000	252.340	0.000	148.828	0.000
ZMAX	1188.000	20.695	610.800	138.897	1165.600	35.514	1016.400	189.233
ST	172.304	29.676	180.478	31.152	174.707	27.031	168.246	27.074
POW	2.000	0.000	2.720	0.330	2.000	0.000	2.000	0.000
FT	19.815	3.633	0.734	0.318	12.746	3.009	9.994	2.320
GW1	39.608	6.903	22.871	6.273	26.711	6.596	16.984	5.729
GW2	25.000	3.500	16.000	3.500	18.250	3.500	13.000	3.500
T	29.280	4.000	24.136	4.000	20.000	4.000	20.360	4.000
S	0.003	0.000	0.004	0.000	0.003	0.000	0.004	0.000

Appendix C: Parameter distributions (mean μ and standard deviation σ) for basins before and after consideration of the scale of model application. The tables show estimated parameters for both the lumped and nodal model applications.

	C12D		C12D_1		C12D_2	
	μ	σ	μ	σ	μ	σ
PI1	0.480	0.034	0.479	0.034	0.480	0.035
PI2	2.964	0.018	2.964	0.018	2.964	0.018
ZMIN	15.095	1.467	40.150	5.480	62.700	24.827
ZAVE	256.936	0.000	314.133	0.000	606.615	0.000
ZMAX	671.800	38.043	682.400	116.038	934.600	133.208
ST	134.265	21.299	177.314	30.935	148.674	27.574
POW	2.900	0.550	2.810	0.420	3.270	0.970
FT	0.637	0.123	0.671	0.197	0.249	0.133
GW	23.000	5.500	20.000	3.500	18.000	3.500
T	40.000	8.000	28.000	2.800	40.000	8.000
S	0.005	0.001	0.005	0.001	0.005	0.001

	K40A		K40A_1		K40A_2	
	μ	σ	μ	σ	μ	σ
PI1	1.964	0.017	1.964	0.017	1.963	0.018
PI2	2.569	0.028	2.571	0.029	2.571	0.029
ZMIN	5.070	1.103	50.000	0.000	71.550	19.025
ZAVE	236.261	0.000	140.258	0.000	328.388	0.000
ZMAX	1160.787	1.005	985.210	1.020	1172.400	26.481
ST	96.751	1.925	137.190	15.898	267.103	39.216
POW	1.980	0.060	2.000	0.000	2.000	0.000
FT	44.156	1.859	11.782	2.808	15.141	2.822
GW	16.330	2.805	30.000	5.000	20.000	3.200
T	40.000	8.000	8.000	0.800	20.000	2.000
S	0.002	0.001	0.002	0.000	0.004	0.000

	K40B		K40B_1		K40B_2	
	μ	σ	μ	σ	μ	σ
PI1	1.963	0.017	1.964	0.017	1.964	0.017
PI2	2.571	0.029	2.572	0.030	2.571	0.029
ZMIN	64.200	4.003	63.150	9.472	54.800	19.383
ZAVE	275.975	0.000	178.004	0.000	228.514	0.000
ZMAX	1155.600	20.613	1194.000	11.547	1168.400	58.478
ST	214.960	24.398	182.277	18.689	230.476	28.739
POW	2.000	0.010	2.000	0.010	2.000	0.000
FT	17.694	5.795	15.660	4.026	14.910	4.132
GW	38.322	4.995	40.000	5.500	30.000	4.500
T	20.000	4.000	20.000	4.000	20.000	4.000
S	0.003	0.000	0.003	0.000	0.003	0.000

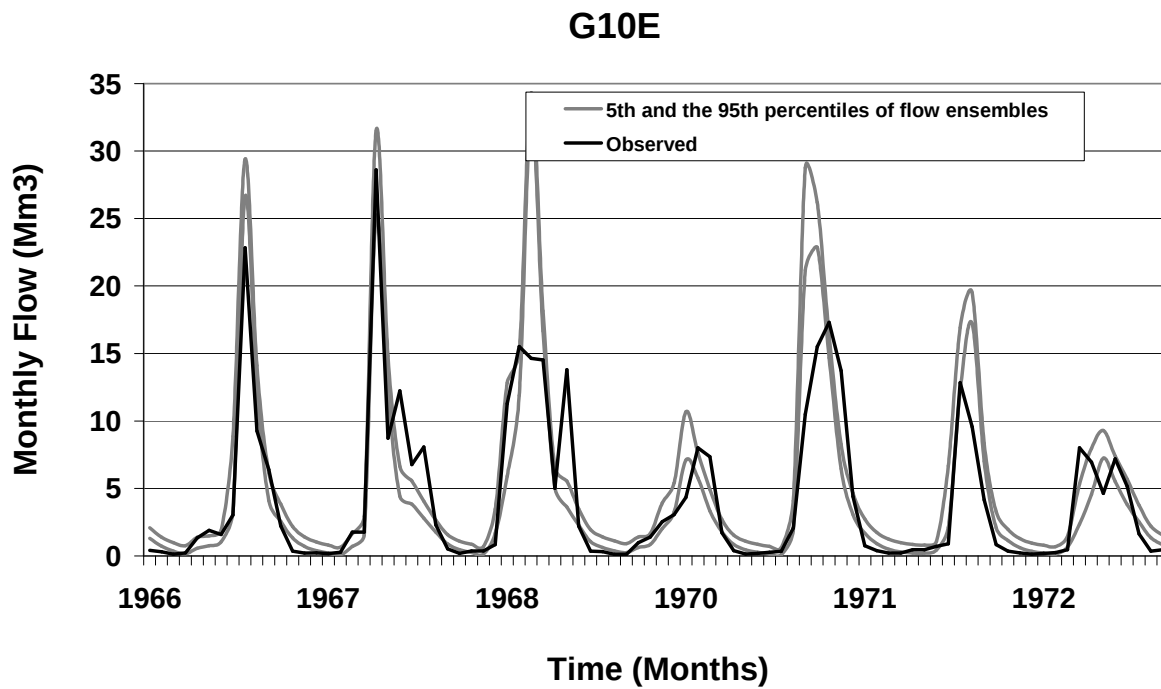
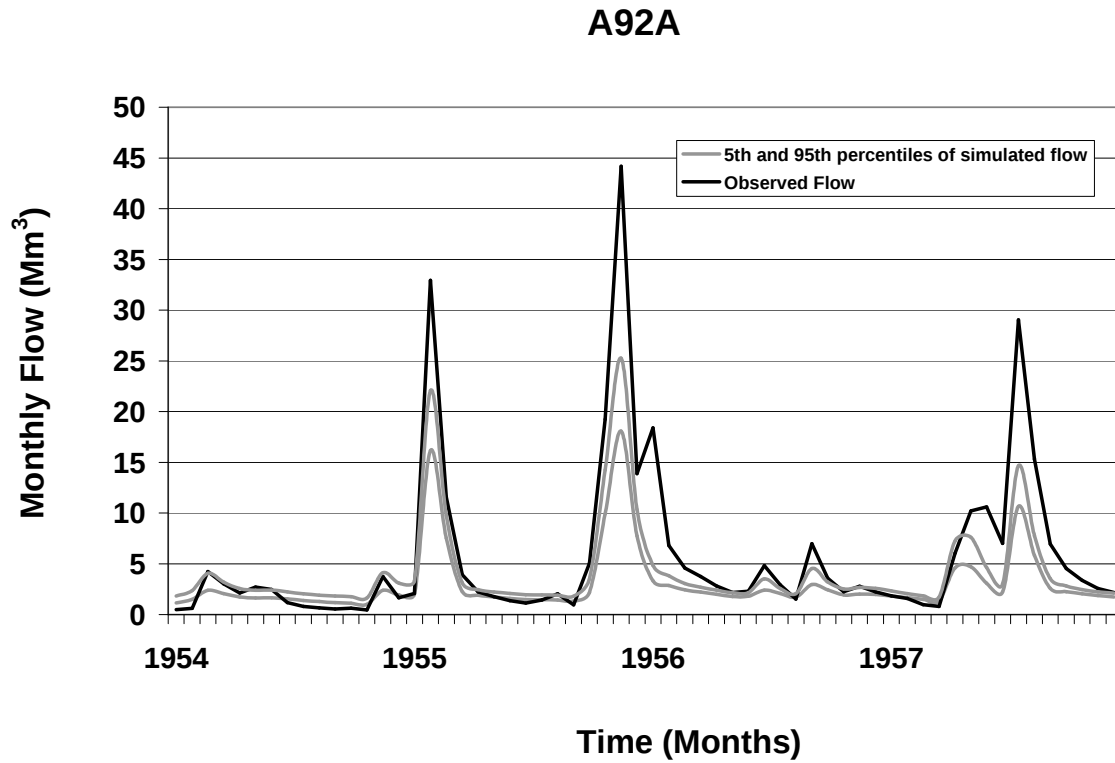
	H10A		H10A_1		H10A_2		H10A_3	
	μ	σ	μ	σ	μ	σ	μ	σ
PI1	0.348	0.022	0.209	0.000	1.119	0.142	0.712	0.096
PI2	2.796	0.017	2.066	0.011	2.772	0.015	2.774	0.016
ZMIN	65.000	0.000	45.000	0.000	60.850	10.102	37.250	10.763
ZAVE	269.384	0.000	82.750	0.000	252.145	0.000	122.420	0.000
ZMAX	1132.000	31.398	800.000	0.000	884.600	25.719	726.000	13.181
ST	160.743	16.129	109.719	18.261	206.755	34.761	141.186	21.763
POW	2.000	0.000	2.000	0.000	2.070	0.250	2.000	0.000
FT	19.895	3.896	7.875	1.380	5.042	2.198	6.008	1.192
GW	13.500	2.250	29.000	5.000	2.000	0.600	15.000	3.000
T	42.400	4.240	50.000	10.000	50.000	10.000	50.000	10.000
S	0.001	0.001	0.001	0.000	0.001	0.000	0.001	0.000

	H10B		H10B_1		H10B_2	
	μ	σ	μ	σ	μ	σ
PI1	0.357	0.022	0.209	0.010	1.134	0.146
PI2	2.882	0.018	2.065	0.011	2.774	0.014
ZMIN	80.000	0.000	65.000	0.000	60.200	26.826
ZAVE	247.970	0.000	348.750	0.000	731.369	0.000
ZMAX	1199.800	2.000	1200.000	0.000	1075.600	93.315
ST	182.565	16.674	165.495	16.259	275.092	55.250
POW	2.000	0.000	1.990	0.030	1.930	0.280
FT	19.068	3.802	24.097	4.839	13.859	7.888
GW	22.500	2.250	32.000	5.000	2.000	0.600
T	40.000	4.000	50.000	10.000	50.000	10.000
S	0.001	0.001	0.001	0.000	0.001	0.000

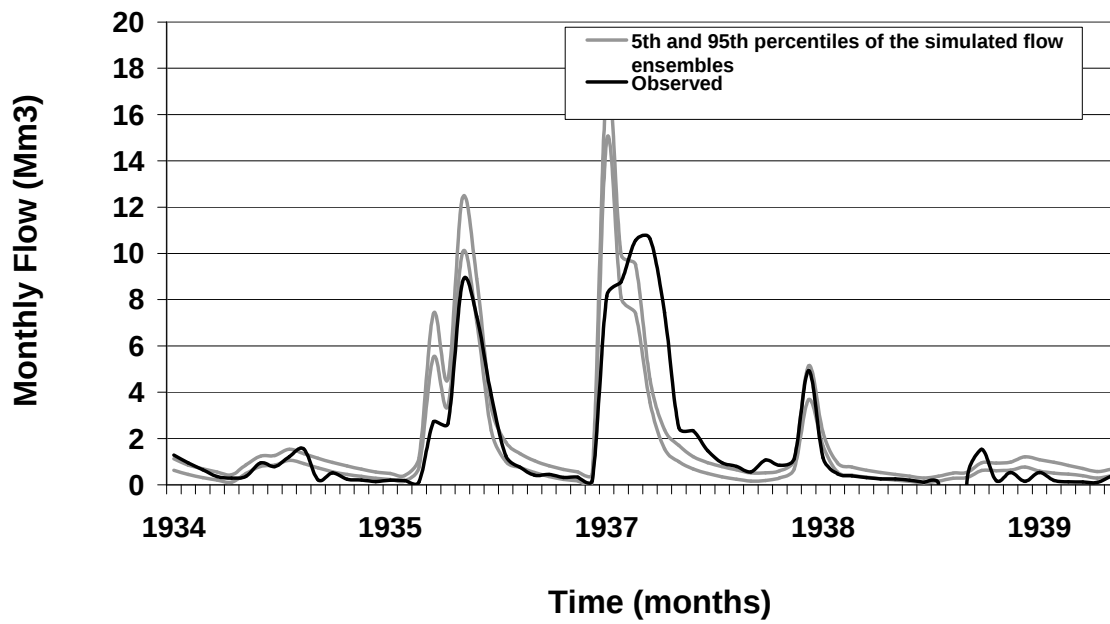
	H10C		H10C_1		H10C_2	
	μ	σ	μ	σ	μ	σ
PI1	0.601	0.067	0.210	0.010	1.124	0.145
PI2	2.348	0.013	2.065	0.012	2.773	0.015
ZMIN	93.600	7.110	65.000	0.000	53.700	19.038
ZAVE	774.178	0.000	292.000	0.000	367.907	0.000
ZMAX	999.600	38.136	1200.000	0.000	1179.200	26.196
ST	166.492	23.261	175.690	17.028	217.111	41.359
POW	1.930	0.100	2.000	0.030	2.460	0.270
FT	36.554	17.428	21.803	7.014	2.408	0.673
GW	15.000	2.000	25.000	4.500	2.700	0.600
T	50.000	10.000	50.000	10.000	50.000	10.000
S	0.001	0.001	0.001	0.000	0.001	0.000

	R20C		R20C_1		R20C_2		R20C_3	
	μ	σ	μ	σ	μ	σ	μ	σ
PI1	1.308	0.116	1.299	0.114	1.231	0.113	1.243	0.115
PI2	3.105	0.019	3.104	0.019	2.952	0.018	2.974	0.017
ZMIN	23.850	11.846	48.800	15.367	21.450	11.085	18.805	1.528
ZAVE	252.340	0.000	129.766	0.000	332.978	0.000	539.744	0.000
ZMAX	1165.600	35.514	896.600	283.129	809.600	52.837	855.000	123.399
ST	174.707	27.031	110.321	18.649	171.270	27.147	208.943	32.213
POW	2.000	0.000	2.000	0.000	3.590	0.810	3.980	0.130
FT	12.746	3.009	13.816	2.989	0.572	0.183	0.494	0.169
GW	18.250	3.500	22.000	2.500	22.000	4.446	20.000	4.500
T	20.000	4.000	20.000	4.000	20.000	4.000	20.000	4.000
S	0.003	0.000	0.002	0.000	0.003	0.000	0.004	0.000

Appendix D: A comparison of the 5th and 95th percentiles (grey graphs) of the simulated ensembles with the time series of observed flow for some selected basins (black graph).



B41G



V20A

