

Decomposition of Groundwater Hydrograph Analysis by Using Time Series

By

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ABSTRACT

Groundwater is one of the most important natural resources in Australia and requires careful and effective management by monitoring the water resources, modelling, and simulating the hydrological process. One of the most important aspects of groundwater modelling is to estimate groundwater recharge and determine the groundwater level fluctuations over a period. Time series analysis is a simple method to analyse groundwater and it is a simple data-driven approach and faster process than a spatially distributed groundwater flow model. This process explains the observed head fluctuation due to different stresses such as precipitation, evaporation, pumping, etc. This time series Transfer Function Noise model is used at the Wagna hydrological research station in south-eastern Austria to analyse the groundwater heads with regular data by the PASTAS. However, sometimes finding consistent data over a long period of time is often challenging. In Australia, where the observed head data series is irregular, this PASTAS technique in Transfer Function Noise modelling with impulse response function has not been attempted. This study applied this PASTAS method on irregular data from 53 wells at the Lower Limestone Coast Prescribed Wells Area, a study site in southwestern South Australia, to determine how the model reflects in terms of groundwater levels and recharge. The study concluded that both the linear and non-linear models worked well to simulate the groundwater head model of the wells in the study area. In case of recharge estimation, the linear model shows more groundwater recharge than non-linear model.

DECLARATION

I certify that this thesis does not incorporate without acknowledgment any material previously submitted for a degree or diploma in any university; and that to the best of my knowledge and belief it does not contain any material previously published or written by another person except where due reference is made in the text.

Signed: Md Mashiur Rahman Talukder

Date: 26 October 2021

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CHAPTER ONE: INTRODUCTION

Background

Groundwater, which is water stored underground in fractures, pores, joints, bedding planes, and cavities of the rock mass, is a vital resource for both the international community and Australia. Globally, groundwater accounts for around 97 percent of all available freshwater on the planet and provides nearly half of the world's drinking and irrigation water (Tello & Hazelton 2018). In addition, groundwater resources in Australia account for 17% of all existing accessible water and up to 30% of water consumption in some regions. With minimal rainfall, high evaporation, and relatively limited surface water supplies, Australia is the world's driest inhabited continent. As a result, groundwater is one of Australia's most precious natural resources, as it provides the only reliable and cost-effective source of water for almost half of the continent's total land area, supporting cities, agriculture, industry, and mining operations (Tello & Hazelton 2018). However, over-extraction of groundwater in combination with increased surface runoff has resulted in groundwater depletion, saline intrusion, and pollution in many areas of Australia. Land clearing for agriculture, livestock grazing, and urbanisation together with over allocation of the groundwater storage have contributed to the lowering of the groundwater table (Frost, Ramchurn & Smith 2018; Gehrels, van Geer & de Vries 1994). In addition to land use changes, climate change and lower rainfall in recent years has further reduced groundwater infiltration and recharge, while higher temperatures have increased evapotranspiration. The cumulative effect on groundwater has been a dramatic reduction in availability of the resource in many places. These declines in groundwater resources have resulted in lower well yields and higher pumping costs, as well as deterioration of water guality, land subsidence, and other negative environmental and socio-economic consequences (White et al. 2016).

Importance of Hydrological Properties

According to von Asmuth and Knotters (2004), the groundwater table and its temporal difference has great impact on the economy, as well as the agricultural and environmental sectors. Thus, it is not surprising that groundwater hydrologists have studied these developments with a view to resolving problems through improved management of the water balance. Information and knowledge about hydrological properties and groundwater fluctuations are required to assess choices of groundwater management policies.

Groundwater abstractions, urbanisation and canalisation of rivers not only effect the nearby groundwater level but also remote areas groundwater level, so managing groundwater effectively is crucial (von Asmuth & Knotters 2004). Groundwater aquifers are extremely complex and heterogeneous systems, posing significant challenges for researchers in groundwater system modelling as well as systematic quantification for sustainable water resource management (Chang et al. 2017). Many external and management-related drivers influence this aquifer state in groundwater management, including precipitation, recharge, discharge, evapotranspiration, extractions, and geological environment, which combined represent the state of the aquifer system (White et al. 2016).

Monitoring water resources, modelling hydrological processes, and simulating the effects of policy measures are all required to develop effective water management. Researchers are being challenged to create methods and tools for monitoring and describing the spatiotemporal dynamics of the hydrological system (Manzione et al. 2010). Precipitation and/or stream flow are frequently used as primary sources in groundwater aquifer modelling. As a result, robust studies are required to determine changes in the groundwater system and to realise the dynamic balance of the abstraction, replenishment, and storage processes in space and time. Sustainable management of groundwater resources is extremely difficult without an understanding of the mechanisms and forces that control the level of groundwater. To pursue sustainable groundwater use, scientific investigations of groundwater discharge with appropriate modelling tools are required, which will aid water managers in developing future groundwater management plans and decision-making processes (Chang et al. 2017).

Groundwater Stresses

The groundwater level can change in response to various stresses that a groundwater system is subjected to. Precipitation is the principal source of recharging in most cases. Surface retention, infiltration, percolation, soil moisture storage, and evapotranspiration are all processes that are difficult to assess as they pass through extremely heterogeneous media. Effective groundwater management often requires separating and identifying the drivers and predicting the water levels under different scenarios. To achieve this, a numerical groundwater model is often developed that requires prior assumptions about the hydrogeology and the dominant drivers. This construction of a model based on prior assumptions can make it challenging to objectively identify dominant drivers and processes (Shapoori et al. 2015b). Decisions involving groundwater management are generally based

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on the projections of aquifer hydraulic characteristics, recharge, and groundwater usage rates. Estimating a realistic groundwater extraction history from limited and infrequent measurement records is a difficult task; however, it is necessary for calculating the impact of extractions on groundwater dynamics and the environment. Four typical methodologies for calculating groundwater utilisation are (1) analysis of energy used for pumping, (2) water budget approach, (3) groundwater hydrograph analysis, and (4) numerical model simulations (Peterson & Fulton 2019).

Different Modelling Methods

WTF

One of the most challenging and important aspects of groundwater modelling is to predict groundwater recharge, or the rate at which aguifers are replenished. The water-table fluctuation (WTF) approach is one of the most extensively used methods in this regard (Healy & Cook 2002). However, it requires knowledge of specific yield and changes in water levels over time. The volume and intensity of precipitation, soil and vegetation types, geology, and terrain all influence recharge rates (Healy & Cook 2002). This method assumes that groundwater levels rise solely because of rainfall recharging the aquifer and recharge can be estimated if the water level rise and specific yield are known. Groundwater levels can fluctuate across a wide range of time intervals. Over decades, both naturally occurring climatic shifts and artificial influences can be responsible for long-term oscillations. The drawbacks of the WTF approach include that the correlation between rainfall and water level is not simple; many places suffer seasonal fluctuations in groundwater levels due to the seasonality of evapotranspiration, precipitation, and irrigation (Crosbie, Binning & Kalma 2005). In addition, this method is only applicable for short-term water table rises, which is caused by individual storms. However, short-term water-table changes can be caused by pumping, or barometric pressure oscillations, among other causes. If rainfall is low intensity and longer duration, recharge may be underestimated; therefore, these factors-induced changes in groundwater level must be considered (Obergfell, Bakker & Maas 2019).

Pumping

Another approach for assessing the flow and storage features of an aquifer, anticipating aquifer reactions to extraction, and estimating the availability of groundwater resources for consumptive use is aquifer testing, also known as pumping or aquifer tests. Aquifer tests are most typically performed to evaluate aquifer parameters and forecast aquifer response

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under various pumping scenarios, such as constant pumping at various production bores and measuring drawdown near the bores (Shapoori et al. 2015a). Aguifer parameters are required to calculate groundwater flow and well capacities, as well as to calculate groundwater recharge. A pumping test consists of removing groundwater in a controlled manner over a period, usually a few days, while measuring the groundwater head in monitoring wells. When the conceptual model is too complex to be given by a mathematical expression, the observed head variations are matched with an analytical model, or with a numerical model (Obergfell, et al. 2013). When a test is performed at a single place, it usually represents the aguifer's overall response to pumping. However, these models have some limitations too. Firstly, according to Shapoori et al. (2015a), pumping tests are costly, and labour expenses are significant, particularly when multiple pumping tests are required over a vast area. Secondly, because these tests are frequently performed over short periods of time (24 and 72 hours), they provide information regarding the aquifer's short-term properties. However, if pumping is done for a longer period, the aquifer's characteristics may provide different results. For example, the aquifer may function consistently for a short time, then may behave differently over time when other factors alter depletion and modify how groundwater responds to pumping. In such cases, pumping experiments over a short period of time will provide information on the aquifer's short-term response, however, if done over several months, the same features can lead to overestimation or underestimation of the long-term drawdown (Shapoori et al. 2015a).

Flood-wave method

The flood-wave approach, which was proposed during 1960s, is comparable to a pumping test in that a single stress disrupts the groundwater head in an aquifer. This technique is appropriate when time-varying precipitation and evaporation have a significant effect on groundwater fluctuations. Analytical response functions provide the same role as the well function in a pumping test, that is, they convert observed head variations to groundwater model parameters via a simple model equation. However, water levels also can be affected by other stresses, such as recharge and evaporation. To address this issue, the effect of each stressor must be determined separately by time series analysis (Obergfell, Bakker & Maas 2016).

Time Series Method

Water managers frequently cite model accuracy as a barrier to using hydrological modelling for operational water management decision-making. The accuracy of hydrological models

depends on the calibration dataset. Data assimilation schemes can be used to update model simulations with available data; however, they often require a great deal of computation. Therefore, data-driven modelling methods are more applicable to replace process-based modelling methods, especially when large amounts of data are available (Pezij et al. 2020). Groundwater time series analysis is a data-driven approach that is significantly faster than using a spatially distributed groundwater flow model. Additionally, it is important to conduct head analysis prior to developing and calibrating a groundwater model. This is the process of establishing a relationship between the measured head in an observation well and the measured stress caused by precipitation, evaporation, and pumping (Bakker & Schaars 2019). It has been widely recognised that groundwater level fluctuation is influenced not only by natural processes, such as precipitation, evaporation, and river water stages; fluctuation is also impacted by anthropogenic activities, such as groundwater abstraction and land use and land cover change. Therefore, it is necessary to detect these drivers and decompose groundwater hydrographs into individual drivers. Hydrograph analysis is one of the simplest and easiest methods to estimate groundwater level fluctuations, to estimate impact of excess pumping for water supply or extraction in an aquifer, to identify linear temporal trends, and to map the potentiometric surface (Shapoori et al. 2015b).

Numerical groundwater flow modelling (MODFLOW) requires prior assumptions of aquifer structures or boundary conditions (Shapoori et al. 2015b). However, calibrating such models is typically difficult, time-consuming, and necessitates major reduction of the ecohydrology and hydrogeology, all of which leads to poor forecast performance. Despite these limitations, hydrograph analysis is beneficial for investigating hydrological dynamics and management scenarios (Peterson & Western 2014).

Importance of Time Series

One of the most important aspects of time series analysis is its ability to decompose hydrograph and estimate individual drivers that influence the aquifer (Shapoori et al. 2015b). Time series models have been shown to provide an empirical way for stochastic modelling, forecasting, and predicting the behaviour of uncertain hydrological systems, as well as for determining the predicted forecast accuracy. When no other data other than hydrological time series are available, or when the extremely variable response of groundwater heads to hydraulic stresses cannot be well described by flow equations, time series models are typically preferred in hydrology over mathematical models. The application of time series models to hydrological time series has been demonstrated to be effective in examining the

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behaviour of groundwater heads over time (Yi & Lee 2004). The purpose of the data-driven modelling is to translate the input signals to output signals. In hydrogeology, it is carried out by groundwater models, which is an analytical or numerical solution of differential equations that describe the flow of groundwater (Bakker & Schaars 2019).

Purpose of Observation well

Hydraulic head variations, also known as hydraulic dynamics, are measured in observation wells to investigate general behaviours of the wells and assess the consequences of water management plans. They can be monitored bi-monthly or yearly, depending on the situation. (Bakkeret al. 2008). Observation wells are installed for a variety of reasons, such as determining seasonal trends of heads, identifying the pattern of the aquifer, and observing the recovery of the aguifer after a significant event, such as drought or rainfall. In observation wells, head values are varied due to several stresses, including rainfall, evaporation, pumping, or barometric variations. A measured head variation is a combination of all the stresses. Sometimes it is difficult to determine which of the stresses has caused the head variation. The information contained in the head time series is a function of the behaviour of the system, and the number of stresses acting in the system and their variation and correlation. For example, head variation could be the result of the increased evaporation in summer due to drought or could equally be the effect of increased pumping for agriculture occurring at the same time in response to lack of rainfall. Therefore, it may be difficult to differentiate between two or more stressors on the groundwater resource (Bakker & Schaars 2019).

Time series analysis requires in-depth knowledge of the subsurface and physical boundary conditions, which cause the flow and take considerable time to develop. These time series analysis simulations are often referred to as white-box, gray-box, or black-box models, which are used to determine the relationship between input and output series without detailed knowledge about the aquifer. The gray-box models are semi physical models and based on a limited number of parameters and predefined response functions, whereas black-box models are statistical models (Bakker & Schaars 2019).

Different Time Series Methods

The advantage of time series analysis is that the measured and modelled head during the whole process are compared until a good fit is obtained. On the other hand, in a regular groundwater model, there may be other factors of poor model fit because of subsurface, spatial heterogeneity, or applied boundary conditions. For example, a time series analysis

for pumping test in a tidal area can extract the pumping response from a measured head series even though it is not visible clearly due to other stresses in the model (Bakker, Maas & Von Asmuth 2008). If no other data than hydrological time series is available, or if flow equations do not adequately represent the extremely variable response of groundwater heads to hydraulic stresses, time series models are usually preferred to mathematical models in hydrology. The use of time series models to analyse hydrological time series has proven effective in investigating the behaviour of groundwater heads over time (Yi & Lee 2004). There are several time series models used to estimate hydraulic dynamics, such as Box-Jenkins (BJ), Autoregressive Integrated Moving Average (ARIMA), Autoregressive Moving Average (ARMA), Periodic Autoregressive (PAR), Transfer Function Noise (TFN) and Periodic Transfer Function Noise (PTFN) models. Many aspects influence the choice of an appropriate modelling approach for a given problem, including the number of series to be modelled, the needed accuracy, modelling expenses, model ease of use, and results interpretation (Khorasani et al. 2016).

Time series models, such as Autoregressive–Moving-Average model with exogenous inputs (ARMAX) require fewer parameters than numerical models and are relatively easy to apply and evaluate, making them suitable for top-down analysis. This type of model has been employed in several research investigations (Shapoori et al. 2015b). To accurately estimate the response of hydrological systems, first described by Box and Jenkins (Box 1970), which analysed the correlation between groundwater level and precipitation surplus is preferable over a deterministic groundwater flow model, such as MODFLOW. This is because constructing an empirical time series model is not only less time consuming but also yields accurate predictions of the hydrological properties (von Asmuth & Knotters 2004). It estimates the Impulse Response (IR) function of the system from the temporal correlation between groundwater level and precipitation surplus time series. The stress series is transformed using IR functions created solely from observation and alternative to complex process-based models. Moreover, TFN modelling does not necessitate prior assumptions on system characteristics and the IR functions provide information on how a water system responds to stresses, such as precipitation, which helps in understanding hydrological characteristics and processes (von Asmuth, Bierkens & Maas 2002). The transfer from infiltration to recharge in the unsaturated zone is linear in this model, and measurements have shown that the water content below the root zone does not vary greatly in temperate climates. Therefore, this assumption is not unreasonable for average soils below the root zone. In an unsaturated zone, transfer functions represent both the delay and smoothing, and this process is considered a black-box process (Besbes & De Marsily 1984).

Model forecasts are stochastic in nature, as shown in Fig. 1.1, which results in their own time series termed 'residuals'. These residuals are generated by errors in the observation process, model parameter errors, model conceptual errors, and model equation evaluation errors. When fitted to the noise model, the residuals are used in estimating the probability of extremes because the deterministic model alone exaggerates the probabilities. In addition, due to the autocorrelation of the signal, the residuals at unobserved time steps can be predicted using the noise model, which can be used for smoothing, forecasting, or updating. These approaches, referred to in the meteorological sciences as data assimilation, make optimal use of both model predictions (von Asmuth & Bierkens 2005).

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Fig 1.1: Systematics of a stochastic model (von Asmuth & Bierkens 2005).

Transfer Function Noise models have been used to simulate time series groundwater level variations; however, the main issue with using them in practice is that the impacts of anthropogenic and natural causes cannot be distinguished. Although residual variation that a model cannot capture is usually insignificant compared to overall variance in groundwater fluctuations, it is usually significant compared to the anthropogenic component, giving the latter a high level of uncertainty. Another reason the TFN models failed to predict groundwater fluctuations is that they assume a linear relationship between input (precipitation and evapotranspiration) and output (groundwater level), which may be non-linear in practice (Berendrecht et al. 2006). The TFN models are also well adapted to

modelling the behaviour and uncertainty associated with events that are not well explained by physical rules alone because they are stochastic. The downside of using TFN models, as described by Box and Jenkins, is that they require a high level of precision from the analyst to use an iterative model identification strategy. Furthermore, because the frequency of all input and output variables is coupled and must be equal, traditional time series models can only be utilised with time series that are equally spaced in time and uninterrupted. An essential downside of this strategy is that the outcomes of the model identification procedure might be confusing, and the process itself is heuristic while also knowledge and labour intensive. Moreover, the model order can be determined automatically using information measures, Bayesian methods, and/or the one-step-ahead prediction error (von Asmuth, Bierkens & Maas 2002).

The Autoregressive-moving-average (ARMA) time series model is effective for estimating non-physical properties and is widely used because of its simplicity and predictability. When applying an ARMA type TFN model to a dataset, the model order, which includes ARMA parameters in both the deterministic and stochastic sections of the model, must be specified. The model order is determined by statistical criteria, such as the cross-correlation function between the explained and explanatory variables. Next, model parameters are calculated using an optimisation algorithm designed to minimise the innovations or one-step-ahead prediction error. If the model does not match the criteria, the process is repeated until the model does. The problem of this model is that the approach used to identify the outcomes model may be ambiguous and labour intensive (von Asmuth et al. 2008).

The advantages of time series models, such as ARIMA, over other physically based, distributed models include their relative accuracy, ease of construction, and established statistical basis. The time series model first considers a physical system as a 'whole'. This is shown in Fig. 1.2, which illustrates how, without needing an explicit specification of the system's complete spatial structure, the effective, overall behaviour of a system at a particular point is modelled (von Asmuth et al. 2012).

Image removed due to copyright restriction.

Fig.1.2: Model system (von Asmuth et al. 2012).

The ARIMA modelling seeks to mathematically characterise a time series and forecast its future trajectory using only the series as a data source. The TFN model can study the relationship of two or more processes, whereas the ARIMA model cannot (Gehrels, van Geer & de Vries 1994). According to Box and Jenkins, the precipitation-groundwater relationship is assumed to be linear with precipitation as a input variable, and groundwater level as the output variable (Changnon, Huff & Hsu 1988). However, the ARIMA model has some drawbacks, one of which is choosing the model order, and there is a danger in projecting uncertainties if no data are available. Obtaining accurate and dependable parameters is challenging when the model is affected by several inputs that do not change over time. Finally, this model is only applicable to linear systems (von Asmuth et al. 2012).

Non-linear time series models, as opposed to linear time series models, can accurately estimate higher groundwater levels, and indicate changes in the degree of saturation in the root zone. Another benefit of using this technique is that natural influences can be distinguished from non-natural influences. However, this model requires a large number of parameters, whereas stochastic models, such as the TFN model, can estimate unknown disturbances, errors due to model assumptions, parameter uncertainty, and inputs, albeit only at shallow water tables (Berendrecht et al. 2006).

TFN model

A new TFN model called the predefined impulse response function in continuous time (PIRFICT) model was developed to overcome several disadvantages associated with discrete TFN models. In comparison to the combined ARX model and Kalman filter, the PIRFICT model extends the possibilities for calibrating TFN models on irregularly spaced time series by not requiring an exponential transfer function (von Asmuth, Bierkens & Maas 2002). It addresses various TFN model drawbacks, such as the utilisation of irregular or high

frequency input and modelling a system with a large memory, without requiring a Box-Jenkins process. It is most commonly used with single input/output series, however it can also handle complex data (von Asmuth et al. 2008).

PASTAS

There were no prior open-source alternative tools before PASTAS to perform Transfer Noise Function modelling based on the impulse response functions in Python (Collenteur et al. 2019). Python is an object-oriented, interpreted programming language that has grown in popularity in science and engineering. Using Python scripts to design groundwater models provides unrivalled versatility and the opportunity to make the entire model construction process transparent (Bakker et al. 2016).

Collenteur et al. (2019) present PASTAS as a program that analyses hydrological time series. It is used for analysing measured heads and estimating groundwater pumping drawdown. The PASTAS project's goals are to build a framework for generating and testing new model concepts and creating ready-to-use software for practitioners. Because these models are analysed using scripts, the entire modelling process becomes visible. The results demonstrate that this model works well for linear processes with groundwater levels that are relatively shallow below the surface. However, in the case of deeper groundwater tables, which are affected by non-linear evaporation and precipitation, further study is required.

Studies have used TFN modelling with PASTAS to determine general information on groundwater characteristics. For example, Bakker and Schaars (2019) showed that time series analysis with PASTAS can be used to determine the variance in groundwater level and using the measured head time series can show how pumping responses can be extracted. Twenty observation wells were utilised in this work to estimate the groundwater aquifer parameters using head response data. In addition, three stresses were used to run the model: sea tidal variation, precipitation, and well pumping discharge. The results showed that PASTAS is a more efficient way than the traditional groundwater model. This method can assist in data cleansing and provide insight into the expected model fit of a standard groundwater model, as well as what processes and stressors should be included in the model. A poor model fit can sometimes imply that there is some stress missing. Furthermore, it can be used to calibrate transient groundwater models as well as offer realistic calibration goals for steady groundwater models.

Furthermore, Collenteur et al. (2021) demonstrated how non-linear TFN modelling may be used to simulate groundwater levels and predict groundwater recharge. The groundwater observed head data from the Wagna hydrological research station in the south eastern region of Austria were utilised to run the model in this study. In comparison to the linear model, the non-linear model provides an excellent simulation of groundwater levels. Furthermore, the TFN model with impulse response functions may be used to predict groundwater recharge. The results also showed that the non-linear function gives more accurate recharge estimates than the linear model, and that the recharge can be estimated in a 10-day timeframe. Model parameters can be acquired by calibrating the model; no prior knowledge of aquifer or soil characteristics is required. This study demonstrates that this approach works on shallow groundwater levels, with consistent and frequent data over time.

Objectives of this study

However, finding consistent data over a long period of time is usually challenging. Sometimes the coverage of head measurements is unequal, and the coverage of head measurements is likewise uneven. Furthermore, measurement frequencies may differ, observation durations may be lengthy or short, and there may be a pause in the recording of observed head data. In Australia, where the observed head data series is irregular, this PASTAS technique in TFN modelling with impulse response function has never been implemented. We'll apply this approach to deep groundwater tables as well.

The goal of this research is to find or quantify a step or a trend in the observed heads because of various stressors such as precipitation and evaporation. Furthermore, in both linear and non-linear models, to determine the contribution of specific stressors to groundwater recharge. The methodology, research area, and study conclusions are provided in the report's following sections.

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CHAPTER TWO: METHODOLOGY

Basics of TFN

According to Collenteur et al., 2019, TFN is used to analyse head time series and determine the cause of head fluctuations due to different stresses, such as rainfall, evaporation, and groundwater pumping, and to quantify the recharge to the groundwater levels.

The basic model of TFN is:

 $h(t) = \sum_{M=1}^{M} h_m(t) + d + r(t)$ (1)

where, h(t)= observed heads

d= base elevation of the model

 $h_m(t)$ = contribution of stress m to head

r(t)= model residuals

The contribution of stress to head can be computed through convolution with a predefined response function θ (t) (von Asmuth, Bierkens & Maas 2002):

$$h_m(t) = \int_{-\infty}^t S_m(\tau)\theta_m(t-\tau)d\tau \dots (2)$$

where, S_m = time series of stress m

 $\theta_{m=}$ impulse response function for stress m

A general used impulse response function is the scale gamma distribution (Collenteur et al. 2019):

 $\theta(t) = A \frac{t^{n-1}}{a^n \Gamma(n)} e^{-t/a} \qquad t \ge 0$ (3)

Where, A= scaling factor

a, n= shape parameter

Γ= Gamma function

Another impulse response function used for pumping is the Hantush Well Function:



For example, Fig: 2.1, Example response functions. (a) Block response to 1 mm/day rainfall. (b) Step response to 1 mm/day of rainfall starting at t = 0 (Bakker et al., 2009)

According to Bakker, Maas & Von Asmuth (2008), to translate the recharge flux into groundwater fluctuations, this four parameter response function can be used:

 $\theta_f(t) = At^{n-1}e^{-t/a-ab/t} \quad t \ge 0.....(4)$

Where, A= scaling parameter

a, b, n= shape parameter

The parameters (A, a, b, n & d) are estimated by the Eq. (1) using the measured data. To determine the recharge model, four parameter or exponential response function can be used and it depends on the hydrogeological setting (Collenteur 2021). In this study, the exponential response function from the precipitation and evaporation data was used to translate the recharge flux into groundwater level fluctuations by using the linear and non-linear model.

Linear model

In the linear model the groundwater recharge is a simple linear function of precipitation and potential evaporation (von Asmuth et al. 2008). This approach can estimate the net

recharge for shallow water levels and in temperate climates with negligible runoff (Zaadnoordijk et al. 2019):

 $R=P-fE_{p}$(5)

Where, R= recharge flux

P= precipitation

E_p= potential evaporation

f= evaporation factor, which is suggested by (Obergfell, Bakker & Maas 2019).

However, it is mentioned as a crop factor (Berendrecht et al. 2003), which 'depends on the soil and land cover' (von Asmuth et al. 2008).

In this approach, there is no storage considered in the root system and the impulse response function must capture the temporal distribution of recharge that may occur as a result of storage in the unsaturated zone (Collenteur et al. 2021). It is also mentioned that the root zone, unsaturated zone, and saturated zone are all represented by the response function.

Non-Linear model

The non-linear model uses the concept of soil-water storage to take the consideration for the temporal storage of water in the root zone (Collenteur et al. 2021). This conceptual model is based on the FLEX (Flux Exchange) hydrological model, which reflects the hydrological processes that take place in the catchments (Fenicia et al. 2006).

This model has two reservoirs: interception and root zone shown in Fig. 2.2. At first, when the precipitated water (P) comes to the interception reservoir, there is some initial evaporation (E_i). After that, when the interception capacity ($S_{i,max}$), i.e., the first reservoir, is exceeded, effective precipitation (P_e) goes to the root zone reservoir. Finally, in the root zone some water is evaporated through transpiration and soil vegetation ($E_{t,s}$). The rest of the water is drained from the root zone to the aquifer, which is known as recharge (R).



Fig. 2.2: Conceptual model for the nonlinear recharge model (Collenteur et al. 2021) Based on the water balance in the interception and root zone reservoir, recharge (R) is calculated as $R=k_s(S_r/S_{r,max})^{\gamma}$(6):

where, k_s = saturated hydraulic conductivity

 S_r = the amount of water in the root zone reservoir $S_{r,max}$ = maximum storage capacity of the root zone reservoir γ = is determining how nonlinear this flux is with respect to the saturation of the unsaturated zone

TFN modelling with PASTAS

A new method for time series analysis is PASTAS, which is an open-source software based on the Python scripting language. It is used for different tasks, such as importing data, constructing models, optimising parameters, and postprocessing the results. It is based on the principle that the analyst has the full control of the modelling process. The design of PASTAS is very simple and object oriented. The Unified Modelling Language (UML) diagrams shown in Fig. 2.3 has three important classes. The main class of the PASTAS code is the Model class, which stores the head series, and keeps track of the stresses, parameters, response functions, constant, and base level settings (Collenteur et al. 2019).

Model StressModel	
oseries stress	
stressmodels rfunc	
parameters parameters	
constant simulate	
noisemodel	
Hoisemodel	
settings RechargeModel	el
settings RechargeModel	el
NoisenfodelsettingsRechargeModelsolverainsimulateevap	el
NoisenfodelsettingsRechargeModelsolverainsimulateevapresidualsrfunc	
NoisenhouelsettingsRechargeModelsolverainsimulateevapresidualsrfuncnoisemodelparameters	

Class Name
Main Attributes
Main Methods

Fig. 2.3: Shows the UML diagrams of the three PASTAS classes outlined in this section

In addition, PASTAS includes the stress model and recharge model which include different stresses, such as rainfall and evaporation. Each type has three classes, which are class name, main attributes, and main methods, as shown in Fig. 2.3.

According to Hutton et al. (2016), scripts ensure consistency and provide a clear summary of the entire modelling process. The author suggested these four steps to improve reproducibility in computational hydrology:

- First, the code is modularised into well-documented functions and classes to make it readable and reusable.
- Second, the use of Python scripts and Jupyter Notebooks ensures welldocumented workflows that can be shared easily.
- Third, the source code is available on a Github repository which provides full version control of the software.
- And fourth, it is possible to refer to specific versions of the code by referring to a PASTAS version.

PASTAS in Python deals with the time series data, and it can convert the irregular steps to regular steps. Collenteur et al. (2019) lists the basic steps for the PASTAS workflow, mainly seven setup processes, which are shown in Fig: 2.4.



Fig. 2.4: The PASTAS model steps

Goodness-of-fit metrics

To evaluate the time series model, goodness-of-fit metrics is a common and independent approach, which is applied to calibrate a solution and is more informative than the average model fit over the entire period (Collenteur 2021). In this study, to evaluate the goodness-of-fit of the simulated groundwater levels and groundwater recharge, there are four metrics used, which are the mean absolute error (MAE), the root mean squared error (RMSE), the Nash–Sutcliffe efficiency (NSE), and the Kling–Gupta efficiency (KGE). The NSE and KGE indicate a good model fit when the value goes towards 1, while for MAE and RMSE when the value approaches zero (Collenteur et al. 2021).

Parameter estimation

By fitting the simulated groundwater levels to the observed groundwater levels, the model parameters are estimated. There are eight parameters needed to estimate for both the linear and non-linear model. The least-square method is used to estimate both model parameters.

The model is run with a different set of parameters and the 95% confidence intervals, which are computed form the simulated recharge fluxes (Collenteur et al. 2021). In addition, all the models were written in Python and are accessible for free as part of the open-source package, and the nonlinear model can be found in the PASTAS library under the name 'FlexModel' (Collenteur et al. 2019).

Study Area

The area of this study was the Lower limestone Coast Prescribed Wells Area (LLCPWA) of south eastern South Australia, which has an undulating coastal plain that slopes to the west and southwest toward the Southern Ocean (Fig: 2.5) (Morgan et al. 2015). The climate of this area is Mediterranean to temperate with hot dry summers and cool wet winters.

Image removed due to copyright restriction.

The groundwater is a significant influencing factor in the LLCPWA area because it has a great influence on industry, agriculture, and ecosystem health in the region. In addition, the majority of the wetlands in this area heavily depend on the groundwater system (Brooks 2010). In the south east of South Australia, groundwater is the link between land management practices, water users, drains and many valuable wetlands, which are regarded as being in a vulnerable position due to the impacts of groundwater depletion (Morgan et al. 2015).

The varying nature of the LLCWPA landscape and the different types of stakeholders bring immense challenges for the water resources management. In 2013, a Water Allocation Plan (WAP) was adopted for the LLCWPA to protect the water resources for all water users, now and in the future (Simmons et al. 2019). However, according to Simmons et al., 2019, the authority was forced to reduce water allocations in 2016, and again in 2018 for all six key groundwater management areas (Coles, Short, Frances, Hynam East, Zones 3A and Zonea 5A) (Fig. 2.6) located in the LLCWPA.

Image removed due to copyright restriction.

Fig. 2.6: Location of the LLCWPA six key groundwater management areas (Simmons et al. 2019)

To investigate this situation in the LLCWPA, this study applied the time series analysis to discover the cause of variation in the groundwater system by analysing different stresses in the area, such as precipitation, evaporation, and extraction.

Data Collection

Data for observation well head measurements were collected from the Government of South Australia website WaterConnect (https://www.waterconnect.sa.gov.au/pages/Home.aspx), which provides the updated information about South Australia's water resources and gives direct access to data (Water Connect 2021). In addition, the daily precipitation and evaporation data was collected from the Bureau of Meteorology (http://www.bom.gov.au), which provides daily precipitation and evaporation data over Australia as a grid interpolated from the different weather stations (Bureau of Metrology 2018). Furthermore, data was collected from the Australian Water Resource Assessment–Landscape model (AWRA-L) version 6.0, which simulates the rainfall and evaporation data at a daily timestep and 0.05° grid (spatial resolution of 25 km²) (Frost, Ramchurn & Smith 2018).

CHAPTER THREE: RESULTS

In this study in the LLCWPA, 53 observation wells were used for running the model which recorded observation head data and stresses, such as evaporation and precipitation, to simulate the model. The locations of the wells are shown in Fig. 3.1, which illustrates the distribution over the whole area.





Apart from being well-distributed over the LLCWPA, the observation wells are located in a diversity of land and land cover types. For example, some are located in forest areas, some are in the populated area, and some are situated in the hilly area. Moreover, the depth of the observation wells varies from 6 m to 218 m, as shown in Fig. 3.2. However, the majority of the wells are at depths of less than 50 m, and only three observation wells (BLA077, KON001, MAC035) have a depth more than 100 m.



Fig. 3.2: Depth variation of the observation wells at LLCWPA

For this study, the model was simulated with data of the period 2010 to 2017 as a calibration period and the three-year period from 2018-2020 as a validation period. A year was also employed as a warm-up period at the start of the model, which is important for the non-linear model because the recharge is dependent on the initial root zone saturation. To simulate the model, the following versions were used for all the observation wells:

Python version: 3.8.5

Numpy version: 1.19.2

Scipy version: 1.5.2

Pandas version: 1.1.3

PASTAS version: 0.17.1

Matplotlib version: 3.4.2

For example, the GAM113 observation well, which is located near the junction of Kennedy Ave, Mingbool Rd, and Fern Rd, is shown in Fig. 3.3. with a depth of around 14.0 m.



Fig. 3.3: A Google Maps satellite image which shows the location of the GAM113 observation well

For the GAM113 observation well, observed head, precipitation and evaporation data are plotted for the model (Fig. 3.4) and all the other observation well data are shown in Appendix: Fig. A1.



Fig. 3.4: Plotted head, evaporation, and precipitation data over time for the GAM113 observation well

Groundwater levels simulated for the GAM113 observation well for the period of 2010 to 2020 are shown in Fig. 3.5. Initial warm-up period for the model was one year before beginning of the simulation, which is necessary for the non-linear model to consider the root zone evaporation. The remaining simulated models are shown in Appendix: Fig A2.



Fig. 3.5: Simulated groundwater levels with the linear and non-linear model for GAM113 well

The model is calibrated for the first seven years from 2010 to 2017, and the last three years are used for validation. For this observation well, both the TFN model (linear and non-linear) shows the same fluctuation in the groundwater level. During the year 2017 the groundwater level was high because there was high precipitation in that year.

The TFN model also estimated the recharge for the GAM113 observation well (Fig. 3.6). It also shows that groundwater recharge is higher in the linear model than in the non-linear model. The trend for recharge is decreasing with time. The recharge estimation for the other observation wells is shown in Appendix: Fig A3.



Fig. 3.6: Recharge model for GAM113 well over the period

After running all the observation wells in PASTAS, the coefficient of determination (R^2) for both the linear and non-linear models was found. If the R^2 value is close to 1 that indicates that the model has a good fit. Accordingly, Fig.3.7 shows the R^2 value for the linear model and Fig.3.8 for the non-linear model for each observation well in the study area.







Fig. 3.8: Coefficient of determination (R²) for the non-linear model for all the observation wells

The results also show the root mean square error (RMSE) for the calibration and validation period. The RMSE values of all the observation wells for both models are shown in Fig. 3.9 and Fig. 3.10, which shows that the validated RMSE is higher than for the calibration period. All the other goodness-of-fit metrics values are shown in the Appendix: Table A1 and Table A2.



Fig. 3.9: Goodness-of-Fit Metrics RMSE for all observation wells (Linear model)



Fig. 3.10: Goodness-of-Fit Metrics RMSE for all observation wells (Non-Linear model)
CHAPTER FOUR: DISCUSSION

The results show that the non-linear model performs better compared to the linear model for groundwater head simulation. This non-linear TFN model uses soil-water storage concepts, which shows good results to forecast groundwater recharge in case of drought conditions. In the Wagna, Austria case study, this model simulated groundwater levels and recharge estimation with more frequent and regular data (Collenteur et al. 2021). In this study in the Lower Limestone Coast Prescribed Wells Area of South Australia, the model used irregular and less frequent data, yet shows similar results. This approach has also been used by several other authors (e.g., Obergfell, Bakker & Maas 2019; Peterson & Western 2014), who found comparable results. However, due to differing conditions, it is difficult to determine the most accurate non-linear recharge model, which requires further investigation.

In this study, observation wells with various ranges of depth from 6 m to 220 m in different parts of LLCWPA, including forest, open field, agricultural, household, and hilly areas, were investigated. The linear and non-linear models were simulated for the recharge estimation over time. For both, the modelled recharge is directly related to the stresses (precipitation and evaporation) and duration of the event for the 10-day interval period used to find the recharge. In the linear model, recharge is higher than in the non-linear model because in the linear model the recharge is calculated using the precipitation and potential evaporation. Moreover, the linear model lacks the ability to temporality store water in the root zone. On the other hand, the non-linear method considers the root zone evaporation which could be the reason for the linear model more applicable recharge estimate for the aquifer.

The results of this study in the LLCWPA show that the model can be run by the TFN method using the predefined response function for shallow to deep observation wells. The Wagna, Austria case study, (Collenteur et al. 2021), showed that the TFN model can be used for the shallow depth (+/- 4m) of groundwater levels. However, this model should be used for a longer period of 10 to 20 years for comparative purposes.

Groundwater recharge is not always the result of groundwater-level fluctuations, since these fluctuations could be the result of other hydrological processes (Obergfell, Bakker & Maas 2019), for example pumping, which can easily affect the model (Bakker & Schaars 2019; Collenteur et al. 2019). Determining the actual recharge may be difficult due to multiple influencing factors for which recorded data can be illusive. For example, in agricultural areas, pumping data may be inaccurate because it is poorly monitored or unavailable due to

anthropogenic factors. Additional processes, such as precipitation entering the system or leaving as surface runoff before penetrating the soil, may be added in the root zone model to make the recharge models usable in varied contexts. Hence, more research in this area of groundwater recharge would be of value.

CHAPTER FIVE: CONCLUSION

In this study, the linear and non-linear TFN model using predefined impulse functions was applied to explore a simple way to analyse the groundwater fluctuations over time with observation head data and different stresses, such as precipitation and evaporation. This model is freely available for the public to use, and enables prediction of the groundwater situation to be done. For this study to the TFN model was used to examine the LLCWPA area, which heavily depends on groundwater. A total of fifty observation wells were studied to calibrate the model and for recharge estimation, which demonstrated that the model can be used with irregular data and deep groundwater levels beyond those explored by other studies. Both the linear and non-linear models worked well to simulate the groundwater head model of the wells in the study area. However, in the case of recharge estimation, the linear model shows more groundwater recharge than non-linear model. It could be happened because of the root zone evapotranspiration or other factors which requires further study to identify the exact reason.

A further finding of the study was that some models did not result in a good fit, which could be due to pumping of groundwater for household purposes or agricultural use occurring coincidentally in the neighbourhood at the time of the study. One limitation in this analysis was that only two stresses (precipitation and evaporation) were used for the model analysis due to the difficulty of capturing data from other factors, which were not available.

Accordingly, further study is needed to analyse the model by examining additional stresses, for example, pumping, or the effect of climate change on the local environment. In addition, determining the consistency of the model with some other existing methods for time series analysis would be of interest, as would identifying the individual contribution of different stresses to groundwater recharge estimation through further exploration of the PASTAS package.

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APPENDICES





























26) GAM061 [₁_p 50 d 25 ل الأل data. E [mm d⁻¹] 4 2 24 E 55.0 54.5 1 2010 2012 2014 2016 2018 2020















32) LKG013









36) MNC005









40) NAN009



44) ROS009









48) WLL007









Fig. A1 Heads, evaporation, and precipitation data over time of 53 observations wells.





52) YOU041



1. BEN017



2. BIN024



3. BIN054



4. BRA020



5. DUF008



6. FOX069







8. GAM003







10. GLE108







12. KON001







14. MIN020







16. MNC005







18. MON035







20. ROS009







22. WAT012







24. WLM010







26. YOU028







^{28.} YOU043

Fig. A2: Simulated groundwater levels in linear and non-linear model







2) BIN024



3) BIN054







5) DUF008



































14) LKG013

15) MIN020



16) MNC005



17) MON008



18) MON035



19) RID010





21) SHT012







23) WLL007







25) YOU026



26) YOU028







Fig. A3: Recharge model for 28 observation wells over the period

	Linear									
OBS_Well		Calibra	tion		Validation					
	MAE(m)	RMSE(m)	NSE(-)	KGE(-)	MAE(m)	RMSE(m)	NSE(-)	KGE(-)		
ARC012	0.23	0.34	0.63	0.7	0.47	0.52	-0.31	0.76		
ARC013	0.21	0.24	0.69	0.71	0	0	0	0		
BEN017	0.31	0.41	0.33	0.53	0.44	0.52	-0.45	0.09		
BEN018	0.37	0.5	0.34	0.41	0.43	0.54	0.39	0.36		
BIN024	0.23	0.27	-0.23	-0.28	0.6	0.61	-113.49	0.37		
BIN032	0.2	0.24	-0.1	-0.44	0.61	0.62	-50.97	-0.41		
BIN053	0.1	0.15	0.59	0.68	0.51	0.52	-12.02	0.51		
BIN054	0.09	0.11	0.2	0.26	0.17	0.18	-28.34	0.4		
BL A002	0	0	0	0	0	0	0	0		
BL A041	0.26	0.3	0.02	-0.05	0.29	0.31	-4.49	0.28		
BL A077	0.18	0.22	0.05	-0.12	0.26	0.27	-11.21	-0.13		
BL A084	0.49	0.64	0.23	0.28	0.3	0.43	0.39	0.42		
BL A085	0.03	0.04	0.58	0.68	0.06	0.08	-1.52	0		
BL A100	0.00	0.01	0.05	-0.08	0.5	0.51	-22.83	-0.87		
BMA006	0.17	0.21	0.57	0.65	0.13	0.01	-0.11	0.35		
BMA008	0.12	0.17	0.57	0.65	0.13	0.10	-0.11	0.35		
BMA010	0.12	0.17	0.57	0.65	0.10	0.10	_0.11	0.00		
BOW004	0.12	0.17	0.57	0.65	0.10	0.10	_0.11	0.00		
BRA020	0.12	0.17	0.07	0.00	0.10	0.10	-0.3	-0.23		
BRA023	0.20	0.23	0.40	0.65	0.47	0.04	_0.0	0.20		
	0.12	0.17	0.37	0.00	0.10	0.13	0.75	0.00		
	0.22	0.23	0.55	0.47	0.15	0.23	-0.53	0.02		
	0.03	0.13	0.00	0.05	0.13	0.2	-0.53	0.0		
	0.2	0.23	0.03	0.00	0.29	0.35	0.54	0.75		
CAM003	0.27	0.55	0.07	0.75	0.30	0.40	0.15	0.00		
GAM061	0.39	0.0	0.14	0.10	0.03	0.00	-0.52	-0.03		
GAM113	0.27	0.20	0.57	-0.33	0.34	0.35	-11.7	0.00		
	0.12	0.17	0.57	0.00	0.30	0.4	-4.11	0.37		
	0.12	0.17	0.57	0.05	0.13	0.13	-0.11	-0.15		
	0.23	0.52	0.50	0.00	0.55	0.03	-1.00	-0.15		
	0.28	0.36	0.34	0.41	0.52	0.54	0 1/	01		
	0.20	0.30	0.54	0.41	0.32	0.04	0.14	0.1		
LING013	0.07	0.1	0.00	0.9	0.21	0.20	-2.03	0.37		
	0.10	0.19	0.02	0.00	0.33	0.33	10.69	0.14		
	0.00	0.09	0.00	0.09	0.71	0.75	-10.00	0.30		
	0.11	0.13	0.0	0.00	0.21	0.23	0.04	1.24		
	0.14	0.10	0.09	0.92	0.20	1.04	-0.73	-1.24		
	0.30	0.01	0.4	0.40	0.62	0.66	-0.03	0.29		
	0.21	0.27	0.52	0.59	0.33	0.00	-2.03	0.09		
	0.12	0.17	0.57	0.05	0.13	0.19	-0.11	0.35		
	0.12	0.17	0.57	0.05	0.13	0.19	-0.11	0.35		
	0.12	0.17	0.57	0.05	0.13	0.19	-0.11	0.35		
	0.23	0.20	0.09	0.70	0.20	0.29	-0.9	0.24		
	0.41	0.52	0.1	0.04	1.12	1.21	-4.95	0.10		
RU5009	0.31	0.41	0.43	0.52	0.42	0.5	0.17	0.29		
511012	0.28	0.41	0.44	0.52	1.13	1.29	-2.00	0.12		
TAT028	0.07	0.09	0.49	0.43	0.3	0.31	-18.14	0.35		
WATUIZ	0.07	0.09	0.74	0.8	0.09	0.12	0.4	0.41		
	0.2	0.26	0.61	0.7	0.22	0.3	0.49	0.61		
	0.1	0.12	0.84	0.89	0.44	0.48	-1.8	0.52		
100026	0.28	0.35	0.62	0.7	0.61	0.79	-0.03	0.37		
100028	0.53	0.69	0.34	0.41	0.5	0.74	0.16	0.31		
YOU041	0.12	0.15	0.69	0.74	0.18	0.21	-0.54	0.1		
1100043	0.76	0.94	-0.01	-0.44	1.05	1.27	-0.17	0		

 Table A1: Goodness-of-fit metrics for linear model

	Non-Linear									
OBS_Well		Calibra	tion	ion Validation						
	MAE(m)	RMSE(m)	NSE(-)	KGE(-)	MAE(m)	RMSE(m)	NSE(-)	KGE(-)		
ARC012	0.23	0.31	0.69	0.75	0.39	0.43	0.1	0.61		
ARC013	0.17	0.23	0.7	0.7	0	0	0	0		
BEN017	0.28	0.4	0.38	0.47	0.36	0.43	0.03	0.17		
BEN018	0.46	0.64	-0.07	0.72	1.1	1.3	-2.5	-0.19		
BIN024	0.28	0.32	-0.74	-0.41	0.66	0.67	-137.69	-0.05		
BIN032	0.05	0.07	0.91	0.88	0.32	0.35	-15.94	-0.61		
BIN053	0.08	0.1	0.79	0.85	0.25	0.27	-2.52	0.33		
BIN054	0.15	0.16	-0.62	-0.41	0.26	0.26	-62.38	0.44		
BLA002	0	0	0	0	0	0	0	0		
BLA041	0.28	0.32	-0.1	0.01	0.25	0.26	-2.93	0.53		
BLA077	0.19	0.23	-0.05	-0.14	0.26	0.27	-11.07	0.22		
BLA084	0.39	0.56	0.43	0.6	0.37	0.44	0.37	0.45		
BLA085	0.02	0.03	0.73	0.79	0.05	0.06	-0.49	0.45		
BLA100	0.13	0.16	0.46	0.35	0.44	0.46	-18.29	-1.08		
BMA006	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
BMA008	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
BMA010	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
BOW004	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
BRA020	0.19	0.28	0.48	0.62	0.4	0.5	-0.14	0.12		
BRA023	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
DUF006	0.18	0.25	0.53	0.66	0.07	0.09	0.96	0.92		
DUF008	0.12	0.16	0.37	0.57	0.11	0.16	0.01	0.65		
FOX069	0.14	0.18	0.9	0.92	0.28	0.36	0.5	0.78		
FOX070	0.2	0.29	0.74	0.83	0.43	0.52	-0.06	0.78		
GAM003	0.39	0.52	0.07	0.13	0.67	0.73	-9.75	-0.34		
GAM061	0.35	0.45	-1.5	-0.2	0.69	0.7	-48.47	-0.24		
GAM113	0.12	0.17	0.55	0.63	0.12	0.16	0.18	0.36		
GGL007	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
GLE108	1.02	1.13	-4.29	-0.32	1.63	1.69	-16.12	-0.84		
HYN001	0	0	0	0	0	0	0	0		
KON001	0.34	0.43	0.09	0.03	0.56	0.59	-0.03	-0.06		
LKG013	0.06	0.08	0.9	0.93	0.2	0.31	0.25	0.23		
MAC035	0.2	0.25	0.39	0.42	0.26	0.3	-1.29	0.52		
MIN020	0.07	0.09	0.85	0.89	0.42	0.47	-3.69	0.08		
MIN028	0.07	0.1	0.91	0.95	0.29	0.3	-0.45	0.65		
MNC005	0.15	0.19	0.88	0.92	0.2	0.2	0.48	0.28		
MON008	0.52	0.78	0.45	0.53	0.87	1.06	-0.08	0.25		
MON035	0.18	0.26	0.4	0.48	0.57	0.68	-2.21	-0.3		
MTB007	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
NAN009	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
PAR033	0.39	0.42	-1.66	0.63	0.47	0.49	-6.76	0.49		
PEN002	0.14	0.17	0.88	0.91	0.27	0.33	-1.46	0.42		
RID010	0.34	0.48	0.22	0.25	0.78	0.9	-2.3	0.13		
ROS009	0.28	0.4	0.46	0.55	0.31	0.44	0.37	0.49		
SHT012	0.26	0.41	0.45	0.54	1.01	1.2	-2.15	0.07		
TAT028	0.04	0.04	0.87	0.93	0.22	0.22	-9.03	0.41		
WAT012	0.07	0.1	0.67	0.8	0.11	0.15	0.01	0.29		
WLL007	0.17	0.24	0.67	0.75	0.16	0.21	0.74	0.75		
WLM010	0.06	0.08	0.94	0.95	0.32	0.36	-0.63	0.76		
YOU026	0.25	0.28	0.75	0.81	0.62	0.84	-0.18	0.38		
YOU028	0.48	0.58	0.55	0.63	0.63	0.76	0.13	0.22		
YOU041	0.09	0.12	0.79	0.83	0.21	0.24	-0.85	0.36		
YOU043	0.48	0.63	0.54	0.67	0.55	0.74	0.6	0.55		

Table A2: Goodness-of-fit metrics for non-linear model