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Calibration of transfer function–noise models to sparsely or irregularly observed time series

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Abstract. A method is presented to calibrate transfer function–noise (TFN) models, operating at the same frequency as the input (auxiliary) variables, to sparsely or irregularly observed time series of the output (target) variable. Once calibrated, the TFN models can be used to predict or simulate the output variable at the same frequency as the input variable. Consequently, the method provides a useful tool for filling in gaps of irregularly or sparsely observed hydrological time series. Although generic and suitable for any type of time series, the method is described through the modeling of a time series of groundwater head data with precipitation surplus (precipitation minus potential evapotranspiration) as input variable. First, the TFN model is written in vector notation, yielding the state equation of a linear discrete stochastic system. Subsequently, the state equation is embedded in a Kalman filter algorithm. The Kalman filter is then combined with a maximum likelihood criterion to obtain estimates of the parameters of the TFN model for small time steps (e.g., 1 day) while using sparsely (e.g., two times a month) or even irregularly observed time series of groundwater head data. The method is illustrated using (subsets of) time series of groundwater head data with varying regular and irregular observation intervals.

1. Introduction

Time series models [*Box and Jenkins*, 1976] are frequently used for the analysis of hydrological time series [*Hipel and McLeod*, 1994]. After calibrating it to a limited series of observations, a time series model may be used for (1) forecasting (real time prediction in time), (2) statistical prediction (predicting the values at nonobserved time steps and estimating the associated uncertainty), and (3) stochastic simulation (simulating realizations of the stochastic process underlying the time series model). These realizations can then be used for uncertainty analysis (as input for another model), for risk analysis, or for some design process. In hydrology, time series models are often preferred over mechanistic models if, apart from the hydrological time series, no other data (such as geophysical parameters) are available. Also, the stochastic nature of time series models makes them very suitable for modeling extremes.

A particularly useful class of time series models are transfer function–noise models (TFN models). Here the hydrological variable of interest or output variable (e.g., discharge from a catchment) is related to one or more input variables (e.g., precipitation intensity, day number) using some deterministic relationship or transfer function. The residual series is then described by a univariate time series model such as an autoregressive–moving average (ARMA(p,q)) model. The deterministic relationship may be linear [*Box and Jenkins*, 1976; *Hipel and McLeod*, 1994] or nonlinear [*Tong*, 1990]. The term "transfer function–noise model" is usually reserved for linear-type models.

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There are several advantages to using TFN models instead of univariate time series models. First, the time series model that is in itself empirical is given a more physical meaning. For instance, a first-order TFN model that relates precipitation intensity to discharge is a discretized version of the well-known linear reservoir. Second, if the output variable shows a trend or a periodicity that is also observed in some of the input variables, these types of nonstationarity are accounted for by the transfer function. This way, there is no need to use complicated nonstationary time series models to analyze the time series of the output variable. Third, when using a TFN model, a time series can be decomposed into several components attributable to different inputs. For instance, discharge variation of a river can be related to both precipitation and a nearby pumping station. This way, it is possible to find out which of the inputs is responsible for an observed trend in the output series. TFN models have been used to model hydrological time series such as groundwater head data [*Tankersley et al.*, 1993; *Gehrels et al.*, 1994; *Van Geer and Zuur*, 1997; *Knotters and Van Walsum*, 1997], stream flows [*Hipel et al.*, 1975; *Chow et al.*, 1983; *Olason and Watt*, 1986], and suspended sediment concentration [*Gurnell and Fenn*, 1984; *Lemke*, 1991].

A disadvantage of TFN models, and of all types of time series models for that matter, is that the time step used depends on the observation frequency of the output variable. For instance, if the discharge of a catchment is observed and recorded only once a day, we are forced to use a 1-day time step (or multiples of that) for modeling discharge time series. Also, time series models require observations of the output variable at regular intervals, which is often not the case. In practice, many hydrological time series have been collected in a more or less haphazard way: An observation is made when an observer happens to be in the neighborhood. Also, it often happens that multiple time series must be analyzed concurrently, while these time series have been collected with different, and often varying, frequencies. Furthermore, it is not uncommon to require information about a hydrological variable at a higher frequency than observed. For instance, the damage to crops due to too shallow water tables depends on the number of consecutive days that the water table level is positioned in the crop's root zone. If the water table depths are observed at a much lower frequency (e.g., in the Netherlands two times a month or sometimes only four times a year), it is impossible to predict yield reductions from these observations. These examples show the need for methods of time series analysis that are able to fill in the gaps of sparsely or irregularly observed hydrological time series.

In many hydrological applications of TFN modeling (e.g., hydraulic head data, stream discharges) the most important input variables used are precipitation or precipitation minus potential evapotranspiration (which we will refer to as precipitation surplus). These input variables are usually observed as daily averages at a large number of locations (e.g., in the Netherlands, rainfall is observed at more than 300 locations and potential evapotranspiration is observed at 24 locations). So if the precipitation surplus is observed as daily averages and the response time of the output variable (target variable) is also of the order of days, it makes sense to model the output variable at time steps of 1 day as well. However, the main problem in using a TFN model with a time step of 1 day, while the output variable is observed with a smaller or irregular frequency, is calibrating the noise part of the TFN model. For instance, if the noise is modeled as an AR(1) process we need the autocovariance function of the residuals. To estimate this from irregularly spaced data is problematic. Also, if the correlation length of the noise process contains only a few observation intervals, estimates of the autocovariance for the shorter lags (1, 2, or 3 days) are likely to be very inaccurate.

In this paper a method is presented to calibrate a class of TFN models operating at the same frequency as the input variable, using sparsely or irregularly observed time series of the output variable. For this purpose the TFN models are first written as a state equation of a deterministic linear stochastic system. This state equation is embedded in a Kalman filter. The Kalman filter is subsequently combined with a maximum likelihood criterion [*Schweppe*, 1973] to estimate the parameters of the TFN model from the sparse or irregularly spaced observations of the output variable. Once calibrated, the TFN model can be used to predict or simulate the output variable at the same frequency as the input variable. Consequently, the method provides a useful tool for filling in gaps of irregularly or sparsely observed hydrological time series. The application that is used to illustrate the proposed method is the modeling of hydraulic head data with daily averages of precipitation surplus as input variable.

The paper is organized as follows. First, a theoretical development of the methods is given. Here the class of TFN models is introduced that is considered in this paper. Also, the state equation of the corresponding stochastic system is derived, and the Kalman filter equations are given, as well as the maximum likelihood criterion of *Schweppe* [1973]. Next, the method is illustrated using a time series of daily observed groundwater head data. Finally, summary and conclusions are given.

2. Theoretical Development

In this section we will develop the theory using the example of groundwater head as output variable and precipitation surplus as input variable.

2.1. Transfer Function–Noise Models

The starting point is a single-output TFN model with the precipitation surplus as the only input:

$$h_t = h_t^* + n_t \tag{1}$$

$$h_t^* = \sum_{\iota=1}^{r} \delta_\iota h_{t-\iota}^* + \sum_{j=0}^{s} \omega_j P_{t-j-b} \tag{2}$$

$$(n_t - c) = \sum_{k=1}^{p} \phi_k(n_{t-k} - c) + a_t + \sum_{l=1}^{q} \theta_l a_{t-l} \tag{3}$$

where

- h_t groundwater head at time step t;
- h_t^* groundwater head at time step t attributable to the precipitation surplus;
- P_t average precipitation surplus between time step $t - 1$ and time step t. P_t is calculated from the average precipitation intensity minus the average potential evapotranspiration calculated according to G. F. Makkink [*Winter et al.*, 1995];
- n_t noise component at time step t which is modeled as a ARMA(p,q) process [*Box and Jenkins*, 1976];
- a_t zero mean discrete white noise process with variance σ_a^2;
- c constant, the expected value of n_t;
- δ_ι autoregressive parameters of the transfer model up to order r;
- ω_j moving average parameters of the transfer model up to order s;
- ϕ_k autoregressive parameters of the noise model up to order p;
- θ_l moving average parameters of the noise model up to order q;
- b delay between input and output.

We will consider only a limited class of TFN models, i.e., those with $r = 1$, $s = 0$, $p = 1$, $q = 0$, and $b = 0$:

$$h_t = h_t^* + n_t \tag{4}$$

$$h_t^* = \delta_1 h_{t-1}^* + \omega_0 P_t \tag{5}$$

$$(n_t - c) = \phi_1(n_{t-1} - c) + a_t \tag{6}$$

A special case of the particular TFN model of (4)–(6) is obtained if the autoregressive parameter of the noise model is taken the same as that of the transfer model, $\phi_1 = \delta_1$:

$$(h_t - c) = \delta_1(h_{t-1} - c) + \omega_0 P_t + a_t \tag{7}$$

Equation (7) is an ARMAX model [*Hipel and McLeod*, 1994, p. 605]. When the constant c is collected on the right-hand side of the equation as $c' = c(1 - \delta_1)$, equation (7) takes the form of a dynamic regression equation [*Knotters and De Gooijer*, 1999].

2.2. State-Space Representation of a TFN Model

The TFN model described by (4)–(6) can be written in vector notation as follows (see *Shea* [1987] and *Van Geer and Zuur* [1997] for a slightly different representation):

$$\begin{bmatrix} h_t^* \\ n_t \end{bmatrix} = \begin{bmatrix} \delta_1 & 0 \\ 0 & \phi_1 \end{bmatrix} \begin{bmatrix} h_{t-1}^* \\ n_{t-1} \end{bmatrix} + \begin{bmatrix} \omega_0 & 0 \\ 0 & c(1-\phi_1) \end{bmatrix} \begin{bmatrix} P_t \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} a_t \quad (8)$$

Using

$$\mathbf{x}_t = \begin{bmatrix} h_t \\ n_t \end{bmatrix} \mathbf{u}_t = \begin{bmatrix} P_t \\ 1 \end{bmatrix} \mathbf{A} = \begin{bmatrix} \delta_1 & 0 \\ 0 & \phi_1 \end{bmatrix} \mathbf{B} = \begin{bmatrix} \omega_0 & 0 \\ 0 & c(1-\phi) \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (9)$$

equation (8) is written as

$$\mathbf{x}_t = \mathbf{A}\mathbf{x}_t + \mathbf{B}\mathbf{u}_t + \mathbf{D}a_t \quad (10)$$

Equation (10) is the state equation of a linear discrete stochastic system.

2.3. Multiple Inputs

The state equation can easily be extended to multiple input series [see also *Shea*, 1987; *Van Geer and Zuur*, 1997]. Suppose that the groundwater head is also influenced by a nearby groundwater abstraction, where the abstraction rates are available at the same frequency as the precipitation surplus. Following (4)–(6), the two-input TFN model of groundwater head is then given by

$$h_t = h_t^* + h_t^{**} + n_t \quad (11)$$

$$h_t^* = \delta_1^* h_{t-1}^* + \omega_0^* P_t \quad (12)$$

$$h_t^{**} = \delta_1^{**} h_{t-1}^{**} + \omega_0^{**} Q_t \quad (13)$$

$$(n_t - c) = \phi_1(n_{t-1} - c) + a_t \quad (14)$$

where Q_t is the average groundwater abstraction between time step $t-1$ and t. The associated linear stochastic system is given by

$$\begin{bmatrix} h_t^* \\ h_t^{**} \\ n_t \end{bmatrix} = \begin{bmatrix} \delta_1^* & 0 & 0 \\ 0 & \delta_1^{**} & 0 \\ 0 & 0 & \phi_1 \end{bmatrix} \begin{bmatrix} h_{t-1}^* \\ h_{t-1}^{**} \\ n_{t-1} \end{bmatrix} + \begin{bmatrix} \omega_0^* & 0 & 0 \\ 0 & \omega_0^{**} & 0 \\ 0 & 0 & c(1-\phi_1) \end{bmatrix} \begin{bmatrix} P_t \\ Q_t \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} a_t \quad (15)$$

Clearly, extending (15) to more than two inputs is straightforward. Also, the state equation can be easily extended to contain multiple output series [cf. *Van Geer and Zuur*, 1997].

2.4. Kalman Filter

The state equation (10) is the basis of the (linear) Kalman filter algorithm. The other important equation is the measurement equation that relates the state to an observation:

$$\mathbf{y}_t = \mathbf{C}_t\mathbf{x}_t + \boldsymbol{\varepsilon}_t \quad (16)$$

where $\mathbf{y}_t$ is a vector of observations, $\mathbf{C}_t$ is a matrix relating the observations to the state, and $\boldsymbol{\varepsilon}_t$ is a vector of random measurement errors. In our case, $\mathbf{y}_t$ and $\boldsymbol{\varepsilon}_t$ are scalars y_t and ε_t and $\mathbf{C}_t$ = [1 1] (equal to [1 1 1] for the two input case). The noise a_t and the measurement error ε_t are both assumed to be zero-mean Gaussian random variables with the following properties (δ is Kronecker's delta):

$$E[a_s a_t] = \delta_{st}\sigma_a^2; \qquad E[\varepsilon_s\varepsilon_t] = \delta_{st}\sigma_\varepsilon^2;$$
$$E[a_s\varepsilon_t] = 0 \qquad \forall\, s, t \in \Re^+ \quad (17)$$

We define the following variables:

- $\bar{\mathbf{x}}_t$ time update: the best linear unbiased prediction of $\mathbf{x}_t$ given the available observations up to and including time step $t-1$;
- $\hat{\mathbf{x}}_t$ measurement update: the best linear unbiased prediction of $\mathbf{x}_t$ given the available observations up to and including time step t;
- $\mathbf{M}_t$ the covariance matrix of the error in the time update: $E[(\mathbf{x}_t - \bar{\mathbf{x}}_t)(\mathbf{x}_t - \bar{\mathbf{x}}_t)^T]$;
- $\mathbf{P}_t$ the covariance matrix of the error in the measurement update: $E[(\mathbf{x}_t - \hat{\mathbf{x}}_t)(\mathbf{x}_t - \hat{\mathbf{x}}_t)^T]$;
- ν_t innovation; difference between the observation and the time update at time step t: $\nu_t = y_t - \mathbf{C}_t\bar{\mathbf{x}}_t$;
- $\sigma_{\nu,t}^2$ innovation variance: $E[\nu_t^2]$.

With the definitions above and the initial conditions $\hat{\mathbf{x}}_0$ and $\mathbf{P}_0$ for $t = 0$, the Kalman filter for the state equation (10) consists of the recursive application of the following equations:

$$\bar{\mathbf{x}}_t = \mathbf{A}\hat{\mathbf{x}}_{t-1} + \mathbf{B}\mathbf{u}_t \quad (18)$$

$$\mathbf{M}_t = \mathbf{A}\mathbf{P}_t\mathbf{A}^T + \mathbf{D}\sigma_a^2\mathbf{D}^T \quad (19)$$

If at time step t an observation is taken,

$$\nu_t = y_t - \mathbf{C}\bar{\mathbf{x}}_t \quad (20)$$

$$\sigma_{\nu,t}^2 = \mathbf{C}\mathbf{M}_t\mathbf{C}^T + \sigma_\varepsilon^2 \quad (21)$$

$$\mathbf{K}_t = \mathbf{M}_t\mathbf{C}^T\{\sigma_{\nu,t}^2\}^{-1} \quad (22)$$

$$\hat{\mathbf{x}}_t = \bar{\mathbf{x}}_t + \mathbf{K}_t\nu_t \quad (23)$$

$$\mathbf{P}_t = (\mathbf{I} - \mathbf{K}_t\mathbf{C})\mathbf{M}_t \quad (24)$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{K}_t$ is a weighting matrix called the "Kalman gain." If at time step t no observation is taken,

$$\hat{\mathbf{x}}_t = \bar{\mathbf{x}}_t \quad (25)$$

$$\mathbf{P}_t = \mathbf{M}_t \quad (26)$$

The Kalman filter as described by (18)–(26) can thus be used to make optimal predictions of the groundwater head with the same time step as the input series $\mathbf{u}_t$, i.e., the input variables P_t or Q_t.

2.5. Estimating Parameters of the TFN Models

The Kalman filter only provides optimal predictions if the parameters of (10) and the variances σ_a^2 and σ_ε^2 are known. However, if the parameters of (10) and σ_a^2 are unknown, they can be estimated from the innovations calculated with the Kalman filter (where σ_ε^2 must be known). Suppose that we have a calibration period with N observations (which may be sparse and taken with irregular intervals) of the output variable and M observations of the input variables. Running the Kalman filter for the calibration period with a parameter set $\alpha^T = (\delta_1, \omega_0, \phi_1, c, \sigma_a^2)$ for the TFN model (4)–(6) or $\alpha^T = (\delta_1^*, \omega_0^*, \delta_1^{**}, \omega_0^{**}, \phi_1, c, \sigma_a^2)$ for the TFN model (11)–(14) gives N innovations ν_t ($i = 1, \cdots, N$) and N estimates of the innovation variance $\sigma_{\nu,t}^2$. These constitute the following criterion:

$$J(N; \boldsymbol{\alpha}) = N \ln (2\pi) + \sum_{t=1}^{N} \ln (\sigma^2_{\nu,t}(\boldsymbol{\alpha})) + \sum_{t=1}^{N} \left(\frac{\nu_t^2(\boldsymbol{\alpha})}{\sigma^2_{\nu,t}(\boldsymbol{\alpha})} \right) \tag{27}$$

Equation (27) equals -0.5 times the log-likelihood function for the innovations of a Kalman filter [*Schweppe*, 1973] under the following conditions: (1) The noise a_t and the measurement error ε_t are Gaussian and obey equations (17), and (2) the Kalman filter is "optimal," which means that its correct parameters are known such that the innovations are independent ($E[\nu_s \nu_t] = 0$ if $s \neq t$). Therefore, given the above conditions, minimizing (27) with respect to α gives a maximum likelihood estimate of the parameters of the TFN model. We used the downhill-simplex method [*Press et al.*, 1986] to minimize (27), because it does not require derivatives of the criterion. The first two terms of (27) are called the bias part of the criterion, whereas the third term, a weighted least squares criterion, is called the observations part [*Schweppe*, 1973]. The bias part is essential for obtaining unbiased estimates of the parameters [*Te Stroet*, 1995; *Bierkens*, 1998].

The covariance matrix of parameter estimation errors can be estimated using the Cramer-Rao lower bound as given by *Schweppe* [1973, chapter 12 and section 14.5]. However, this method only provides a first-order estimate, assuming small estimation variances and no estimation bias. In our case we did not need to use such an approximation. Indeed, because of the small dimensionality of the stochastic system considered, it is feasible to obtain the statistics of the parameter estimation errors through a Monte Carlo analysis: Using the estimated parameter set and the TFN model, a sufficient number (a least 30) of realizations of groundwater head data are simulated. From these realizations, only the data are retained for the days at which in the original data set the output variable has been observed. Next, the calibration is performed for each of the simulated sets of observations. This results in as many estimated parameter sets as simulated realizations. From these parameter sets the error statistics, such as the covariance matrix, of the parameter estimates can be estimated.

2.6. Summary of Method

In summary, suppose that we are modeling a time series of output data using a TFN model (equations (4)–(6) or (11)–(14)) with daily observed input variables. On the basis of the daily frequency of the input variables we aim to use a time step of 1 day, even though our output data may be sparsely or irregularly sampled in time. First, the TFN model is written as a state equation in vector notation (equation (8) or (15)). The state equation is embedded in a Kalman filter (equations (18)–(26)). By running the Kalman filter for some parameter set $\boldsymbol{\alpha}$, a maximum likelihood criterion can be evaluated with the filter innovations and innovation variances. Minimization of this criterion with respect to the parameter set $\boldsymbol{\alpha}$ gives the (unbiased) maximum likelihood estimates of the parameters of the daily TFN model.

3. An Example Application

3.1. Description of the Data Set

The method is tested using a 15-year (1981–1995) time series of groundwater head data observed with a frequency of one observation per day (taken at approximately 9:00 A.M.). This time series is divided into two sets. One set covering the period 1981–1990 is used for calibration, and the other, covering the period 1991–1995, is used for validation. The time series is obtained from an observation well located on the main meteorological field of the Royal Netherlands Meteorological Office at De Bilt. De Bilt is a small town located in the center of the Netherlands near the city of Utrecht. The meteorological field lies at the edge of an ice-pushed ridge that is a remnant from the glaciers that covered the north of the Netherlands during the Saalien ice age. Because of its proximity to the ice-pushed ridge, it is expected that the groundwater head fluctuation at the meteorological field depends not only on the local precipitation surplus but also on a regional groundwater flux from the higher parts of the ridge. In this study the TFN model only uses precipitation surplus as an input variable. Therefore it can be expected that the influence of the regional groundwater flux is contained in the noise model (i.e., in the parameters ϕ, c, and σ_a^2). In accordance with the Dutch meteorological standard, the land use is grassland. The precipitation surplus is obtained from daily averaged observations of precipitation and potential evapotranspiration at the meteorological field.

3.2. Calibration With Varying Observation Frequency

From the time series of groundwater head data of the calibration period, subsets of observations are selected with decreasing observation frequency. This results in eight series of observations covering the 10-year calibration period with the following regular intervals Δt (days) between observations: 1, 3, 7, 10, 15, 30, 60, and 90 days. Also, 240 observations are selected at random day numbers according to a Poisson process. The latter set of observations is not only sparse (on average, 24 observations per year) but also extremely irregular in time.

A TFN model with a time step of 1 day is calibrated to each of the nine subsets of observations using the methods described in the previous section. In accordance with Box-Jenkins time series modeling, it is assumed that no observational errors are made: $\sigma_\varepsilon^2 = 0$. Figure 1 gives an example of the Kalman filter time updates of the TFN model after calibrating it to the set with observation intervals of 15 days.

Table 1 lists the nine parameter sets obtained from calibrating the TFN model to each of the nine subsets of observations. The number of observations given for the subsets with regular intervals is a little smaller than expected (e.g., one expects 3652 observations for 1981–1990 if $\Delta t = 1$, instead of 3180). The reason is that for almost 9% of the days no observations were available (values are missing). In Table 1 the standard deviations of the parameter estimation errors are given in parentheses. These standard deviations are obtained through a Monte Carlo analysis (see section 2) using 100 realizations.

Table 1 shows that similar values are obtained for the parameters δ_1, ω_0, and c for observation intervals up to 60 days, as well as for the set of the random observations. As expected, the standard deviations steadily increase with decreasing observation frequency. The results for the noise parameters ϕ_1 and σ_a^2 are less consistent. A slight drift of σ_a^2 is observed. The standard deviations show a steady increase for observation intervals up to 15 days and a larger jump from 15 to 30 days. When compared with its estimated value, the large standard deviation of σ_a^2 indicates that an observation interval of 30 days is too large to properly identify σ_a^2.

A more general statement can be made about the minimal observation frequency required to estimate the parameters of the TFN model. The parameters δ_1 and ϕ_1 are the lag-one

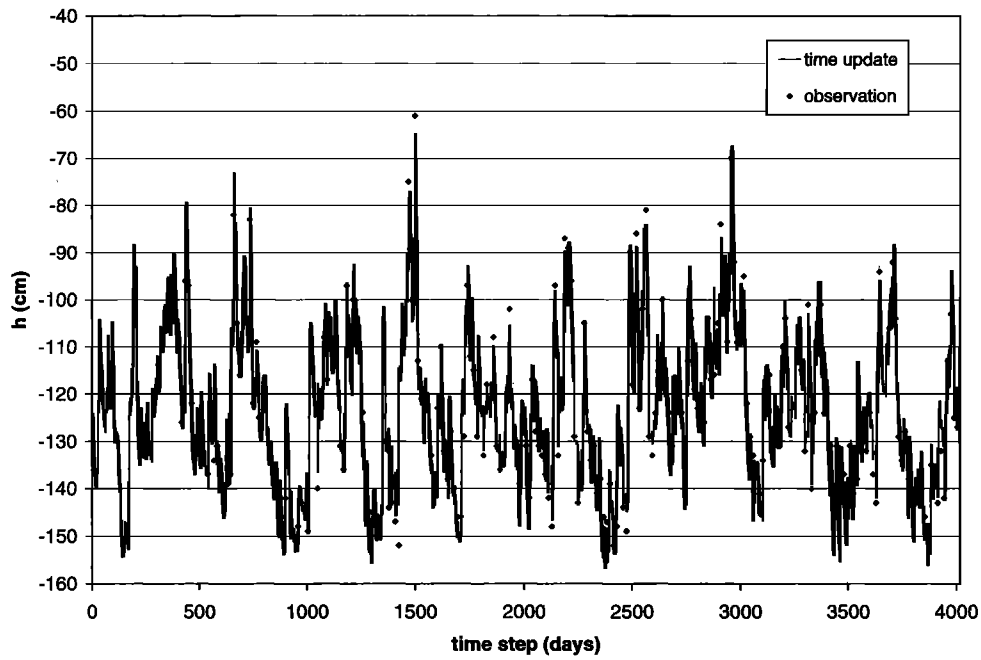

Figure 1. Kalman filter time updates of the transfer function–noise (TFN) model and observations for the period 1981–1990. The TFN model is calibrated to the set with observation intervals of 15 days.

correlation of h_t^* (for random input) and n_t, respectively. In order to estimate them, these correlation coefficients should therefore be reflected in the observations of h_t^* and n_t. This entails that observation intervals should not exceed the characteristic response times of h_t^* and n_t, i.e., the time it takes for a system to reach its equilibrium after a change of input. The characteristic response time λ [T] of a first-order difference equation such as (5) can be found by noting that its impulse response (or in case of equation (6) its correlation function) has an exponential form, i.e., $u(s) = \exp(-s/a)$, where $u(s)$ is the impulse response, a is its parameter, and t is time in days. With δ_1 equal to $u(s = 1)$ we have $a = -1/\ln(\delta_1)$. The impulse response reaches zero asymptotically. For this reason a so-called effective characteristic response time (effective range) is used. The effective characteristic response time is usually taken as $s = 3a$ for which $u(s)$ is just smaller than 0.05 (compare *Deutsch and Journel* [1992, p. 23] for the effective range of an exponential variogram). So the characteristic response time for difference equation (5) becomes

$$\lambda = \frac{-3}{\ln(\delta_1)} \tag{28}$$

Taking the value for δ_1 calibrated for $\Delta t = 1$ day, it follows that the characteristic response time of h_t^* equals 61 days. Similarly, using ϕ_1 for $\Delta t = 1$ day in (28), the characteristic response time for n_t equals 26 days. These values are close to the maximum observation intervals derived from Table 1. The minimal observation frequency required for δ_1 also applies to ω_0 because the estimation errors of these parameters are strongly correlated. The minimal observation frequency required for ϕ_1 also applies to σ_a^2 for the same reason. As shown by the estimated values and the standard deviations in Table 1, the parameter c (the average level of the output variable) is not sensitive to the observation frequency.

3.3. Validation: Predictions

Equation (5), i.e., the deterministic part of the TFN without the use of the Kalman filter, is used to predict the groundwater head on a daily basis for the validation period 1991–1995 using each of the nine calibrated parameter sets. Figure 2 shows such predictions using the parameters for $\Delta t = 15$ days together with observations. Also shown are the 95% prediction intervals, which can be estimated from the noise parameters as

Table 1. Estimated Parameters of the Transfer Function–Noise Model Resulting From Calibrating the Model to Hydraulic Head Series Observed With Decreasing Frequency and a Random Frequency

Δt, days	N	δ_1	ω_0, day^{-1}	ϕ_1	c, cm	σ_a^2, cm^2
1	3180	0.9523 (0.0024)	4.705 (0.13)	0.8940 (0.0050)	−130.3 (0.67)	17.43 (0.43)
3	1060	0.9527 (0.0027)	4.947 (0.19)	0.8890 (0.0080)	−130.7 (0.65)	18.02 (0.82)
7	500	0.9480 (0.0034)	5.401 (0.24)	0.9105 (0.0086)	−130.5 (0.78)	15.08 (1.15)
10	318	0.9420 (0.0043)	5.733 (0.28)	0.9288 (0.0083)	−130.2 (0.81)	11.60 (1.23)
Random	240	0.9447 (0.0054)	5.486 (0.37)	0.9386 (0.0097)	−130.6 (1.15)	11.82 (1.25)
15	210	0.9427 (0.0052)	5.226 (0.38)	0.9220 (0.015)	−129.9 (0.85)	13.52 (2.12)
30	106	0.9453 (0.0068)	5.185 (0.53)	0.9205 (0.064)	−129.7 (0.89)	13.11 (9.23)
60	52	0.9537 (0.0075)	4.606 (0.61)	0.8269 (0.080)	−129.1 (1.19)	26.76 (7.26)
90	35	0.9579 (0.0098)	3.502 (0.70)	0.9102 (0.060)	−129.7 (1.57)	11.75 (5.36)

The random frequency was, on average, two times per month.

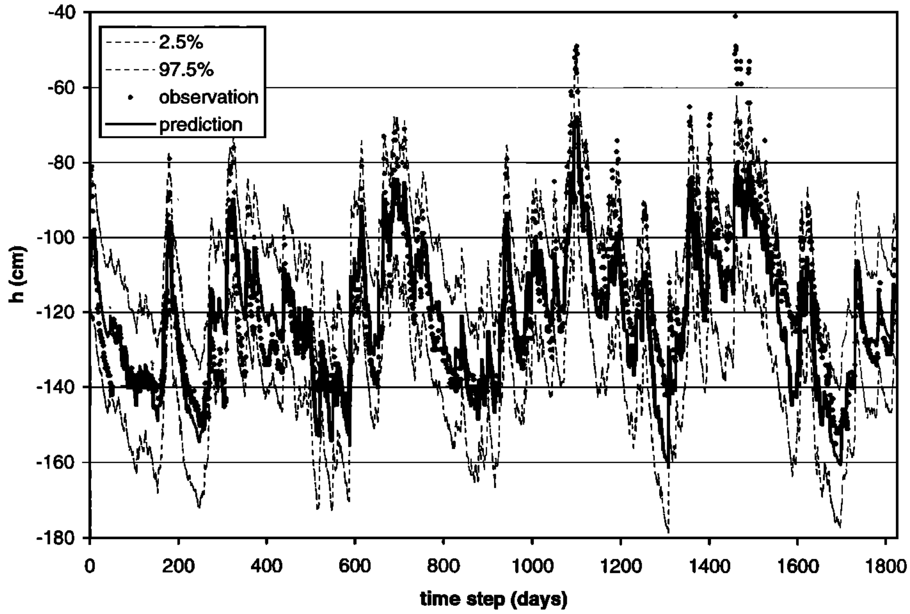

Figure 2. Predictions and 95% prediction intervals of hydraulic head for the period 1991–1995 shown together with the observations. The TFN model is calibrated to 1981–1990 with observation intervals of 15 days (see Table 1 for parameters).

$$\left[h_t^* - 1.96\sqrt{\frac{\sigma_a^2}{1-\phi_1^2}},\ h_t^* + 1.96\sqrt{\frac{\sigma_a^2}{1-\phi_1^2}}\right]$$

The predictions for the validation period are compared with the observations by calculating the mean error (ME) as a measure of bias, the root-mean-square error (RMSE) as a measure of accuracy, and the mean absolute error (MAE), also a measure of accuracy but less sensitive to large errors than the RMSE.

The results of validating the TFN model with predictions using the different parameter sets are shown in Figure 3. It can be seen that equally good predictions are obtained with parameter sets calibrated with observation intervals of less than 60 days. At 60 days the ME starts to fluctuate and the RMSE and MAE start to increase. The predictions of the models calibrated to the random subset show a little more bias but are equally accurate as the results obtained from regular intervals.

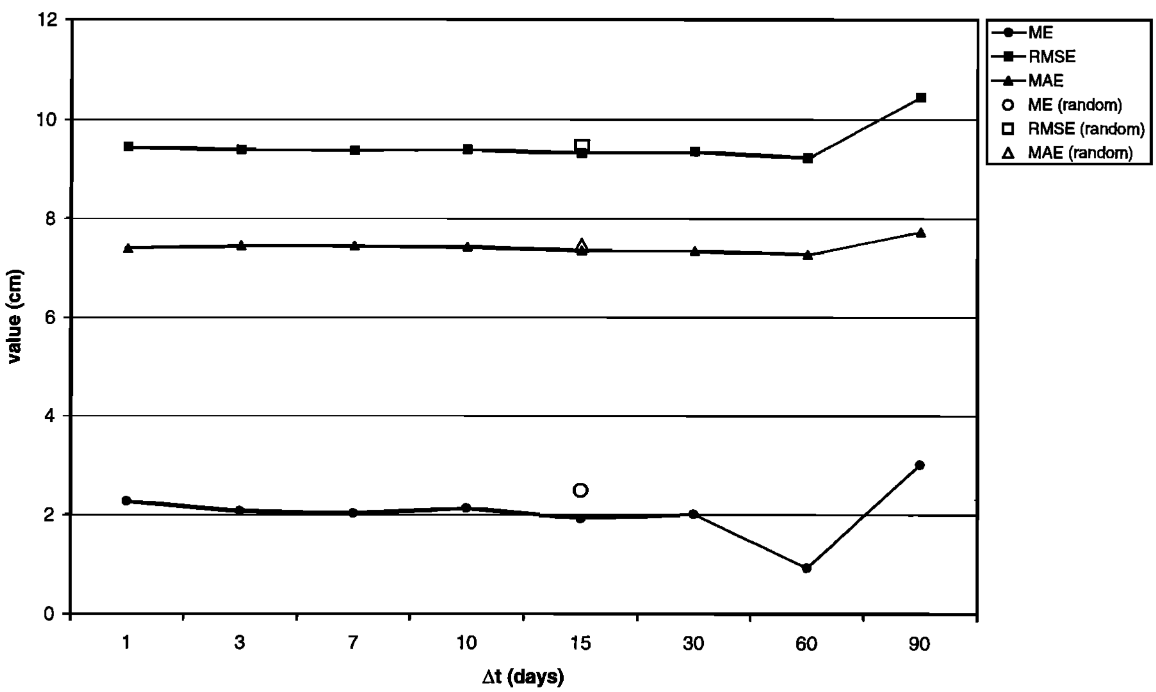

Figure 3. Statistics of comparing predictions with the TFN model with observations for the period 1991–1995. The TFN model is calibrated to subsets of 1981–1990 with increasing regular observation intervals and a subset of 1981–1990 with random observation intervals.

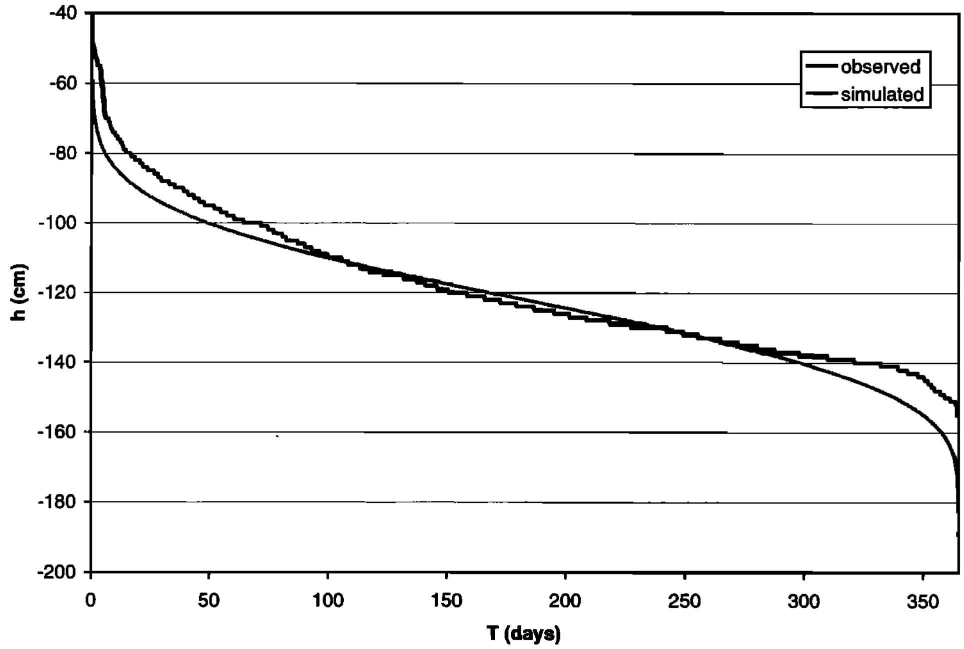

Figure 4. Frequency of exceedance (FOE) graphs of hydraulic head for the period 1991–1995 as estimated from the observations and estimated from 1000 realizations simulated with the TFN model. The TFN model is calibrated to 1981–1990 with observation intervals of 15 days.

3.4. Validation: Statistics From Stochastic Simulation

Using (4)–(6), for each of the nine parameter sets, 1000 realizations of daily groundwater head data are simulated for the validation period. For each of the parameter sets the following statistics are estimated from the 1000 realizations.

First is the frequency of exceedance graph (FOE graph). A FOE graph gives for each value of the groundwater head the expected number of days per year that this value is exceeded. A FOE graph thus represents the cumulative probability distribution of groundwater head. It must be noted that the FOE graph is estimated using the simulated data of all 1000 realizations at once. This means that the FOE graph represents the first-order ensemble statistics of the stochastic process h_t, representing both uncertainty and variation with time.

Second is the correlation function. The correlation function of the stochastic process that is generated by the TFN model (with the given parameter set) can be estimated from the 1000 realizations as follows: First, for each realization the correlation function is estimated. Then the correlation function of the stochastic process is estimated by averaging for each lag the values of all the 1000 correlation functions of the realizations.

The FOE graphs and correlation functions obtained from the model simulations are compared with the FOE graph and correlation function estimated from the observations in the validation period. Comparison is done by calculating from the differences the ME, RMSE, and MAE. These measures show how well the first- and second-order statistics of the observations in the validation period are described by the first- and second-order statistics of the stochastic processes generated by the TFN model with the given parameter set. As an example, Figure 4 shows the FOE graph estimated from the observations and the 1000 realizations simulated with the TFN model after calibrating it to the set with an observation interval of 15 days. Figure 5 shows the correlation functions.

Figure 6 gives the results of validating the first-order statistics (i.e., the FOE graph) estimated from 1000 realizations simulated with the TFN model for the various parameter sets. It can be seen that the first-order statistics are reproduced well for parameter sets belonging to observation intervals less 60 days. When compared with regular observation intervals of 15 days, results for random observation intervals are almost equal. Figure 7 shows the validation results of the second-order statistics (correlation functions). We can see that similar results are obtained for all parameter sets. Figure 7 also shows that the results for random observation intervals are the same as for the regular observation interval of 15 days. Note from the validation of the statistics that although the noise parameters are poorly identified from observation intervals of 60 days, the TFN model is still able to reproduce the statistics with these parameters.

4. Summary and Conclusions

The goal of this paper was to develop a method to calibrate a class of transfer function–noise (TFN) models, operating at the observation frequency of the input variables, to sparsely or irregularly observed time series of the output variable. To achieve this, the TFN model was first written in a vector representation. This representation yielded the state equation of a linear discrete stochastic system and was subsequently embedded in a Kalman filter. Parameter estimates of the TFN model could be obtained when the Kalman filter was combined with observations of groundwater head data (which may be sparse or irregular) and a filter-type maximum likelihood criterion [*Schweppe*, 1973]. When calibrated, the TFN model can be used to predict or simulate the output variable at the same frequency as the input variable. Consequently, the method provides a useful tool for filling in gaps of irregularly or sparsely observed hydrological time series.

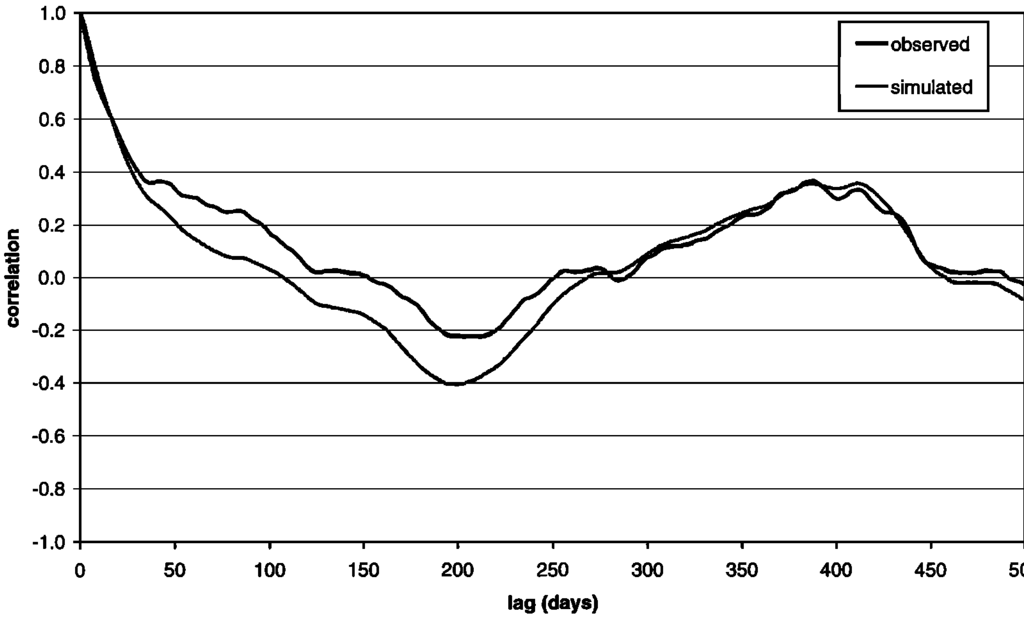

Figure 5. Correlation functions of hydraulic head for the period 1991–1995 as estimated from the observations and estimated from 1000 realizations simulated with the TFN model. The TFN model is calibrated to 1981–1990 with observation intervals of 15 days.

The proposed procedure was illustrated with a calibration and validation study using 15 years (1981–1995) of daily observed groundwater head data from a piezometer at the meteorological field of the Royal Netherlands Meteorological Institute. The TFN model was first calibrated to subsets of observations with increasing observation intervals selected from the first 10 years (1981–1990). After that the calibrated models were validated by comparing predictions and statistics from stochastic simulations with daily observations for the years 1991–1995. The same procedure was followed while using a subset of 240 randomly selected observations from the period 1981–1990 as calibration data.

On the basis of the calibration and validation study the following conclusions were drawn for the data set analyzed:

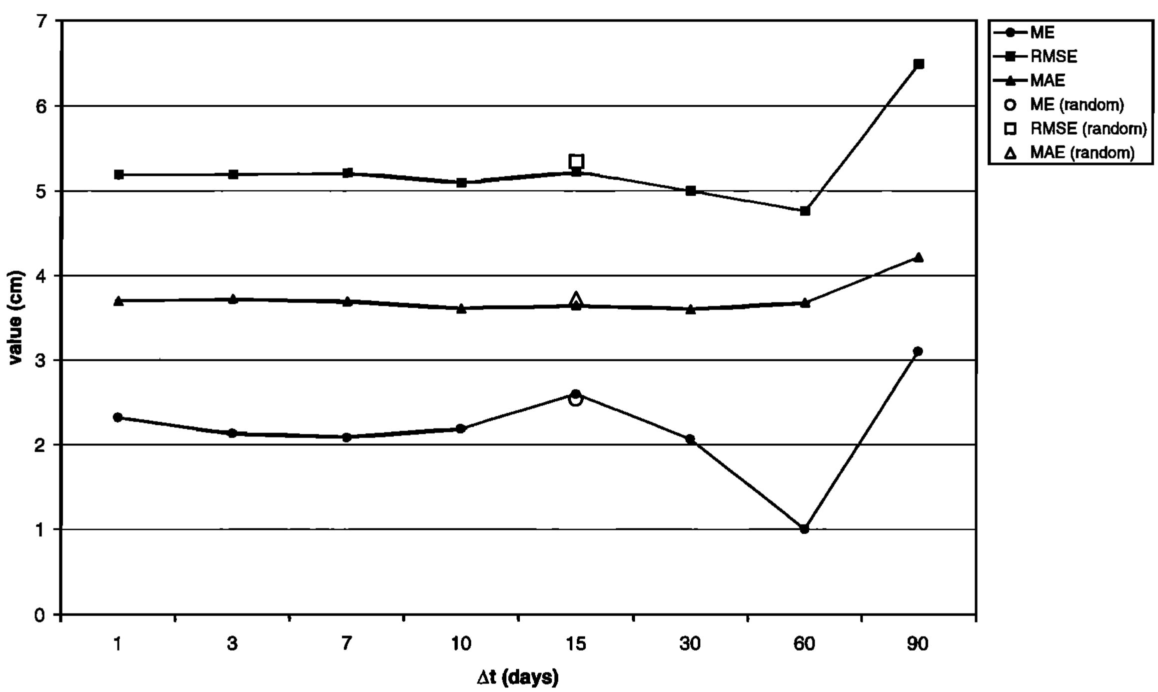

Figure 6. Statistics of comparing FOE graphs estimated from 1000 realizations simulated with the TFN model with the FOE graph estimated from the observations (period 1991–1995). The TFN model is calibrated to subsets of 1981–1990 with increasing regular observation intervals and a subset of 1981–1990 with random observation intervals.

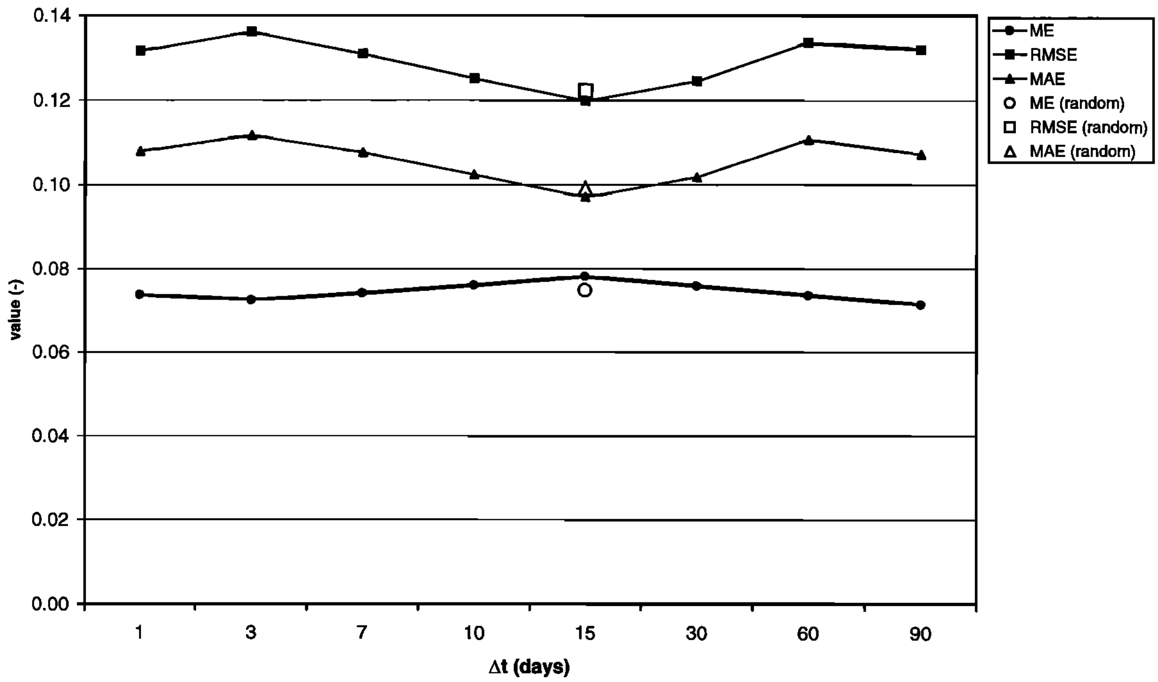

Figure 7. Statistics of comparing correlation functions estimated from 1000 realizations simulated with the TFN model with the correlation function estimated from the observations (period 1991–1995). The TFN model is calibrated to subsets of 1981–1990 with increasing regular observation intervals and a subset of 1981–1990 with random observation intervals.

1. Similar parameter values are obtained for the transfer function part of the TFN model for observation intervals less than 60 days and for the noise part of the TFN model for observation intervals less than 30 days. These results are in accordance with the characteristic response times of the transfer function and the noise model, respectively.

2. The TFN model yields accurate predictions and representative stochastic simulations of daily groundwater head data as long as the model is calibrated to data sets with regular observation intervals less than 60 days.

3. The results obtained from calibrating the models to a data set with random observation intervals are comparable to the results obtained for regular observation intervals with the same average frequency.

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