Improved Simulation With Linear and Nonlinear Reservoir Models Using Optimal Estimation Theory

by

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Abstract

Optimal estimation theory (Kalman Filter) is applied to linear and nonlinear reservoir conceptual models of hydrologic systems. The filter algorithm for the nonlinear reservoir is derived using a Taylor series expansion about the value of storage at the current time step. Thus, the state transition matrix is constant for a linear reservoir, whereas for the more general case of a nonlinear reservoir, it is a function of the reservoir storage at each time step. Examples using hypothetical data illustrate the relative importance of measurements of inflow, outflow, and storage in improving model predictions. If only two variables could be measured, one should always be storage, regardless of which of the three state variables is being considered. The reduction of variance (uncertainty) in predicted and measured values of the state variables using the filtering technique is illustrated in examples for both linear and nonlinear reservoirs.

INTRODUCTION

The union of conceptual reservoir modelling and optimal estimation theory provides several benefits over conventional reservoir modelling alone. First, the estimates produced by filtering data each time step are better (smaller variance about the unknown true value) than are predictions from the reservoir model alone. Second, additional information is available from the filter estimate about the variance of all state variables. This objective measure of certainty is invaluable when the estimates are used in making economic decisions. For example, if in a flood situation the estimate of reservoir inflow were used to determine whether to (a) evacuate a town, (b) shore up levees, (c) move livestock and equipment, or (d) do nothing, a measure of the certainty of the outflow estimate (i.e., the variance) must be considered to make a sound judgement.

Another benefit of the union of conceptual modelling and filtering is the view of the world which results. A conceptual model (typically physically based) produces an estimate of the true state of the system being modelled. This estimate is known to be in error due to modelling errors, input errors, and random errors resulting from predicting using expected values of the stochastic components of the system. Measurements of the states are made. These measurements are estimates of the true states corrupted by measurement error. The two estimates (model and measurement) are combined so as to use all available information and minimize the error of the resulting estimate.

THEORETICAL BACKGROUND

Simple reservoir equations have been used as a conceptual model of the movement of water for many years in the field of hydrology (Zoch 1934, 1936, 1937; Horton 1938; Nash 1958; Dooge 1973). Both linear and nonlinear reservoirs have been used to conceptualize rainfall/runoff relationships, streamflow, and urban runoff elements. The reservoir equations may be simply stated as:

$$Q = k\, S^{\alpha} \tag{1}$$

and

$$\Delta S = I - Q \tag{2}$$

where Q = the outflow from a reservoir,
k = an empirical constant (known as the reservoir constant),
S = the storage in a reservoir,
ΔS = the change in storage,
I = the inflow to a reservoir, and
α = an empirical coefficient.

Discussion of modelling systems as reservoirs generally falls into two categories: linear ($\alpha = 1$) and nonlinear. This paper will begin by deriving results for the linear reservoir case, but will later show that the linear can simply be treated as a special case of nonlinear reservoir modelling, the objective being to link the existing hydrologic knowledge of

conceptual reservoir models with the body of knowledge known as optimal estimation or filtering theory. This union will result in better estimates of the reservoir inflow, storage, and outflow than are available from conceptual reservoir modelling alone. The phrase "better estimate" is used above to mean an estimate that has a smaller variance about the true value of inflow, storage, or outflow than estimates from reservoir models alone.

The point of view on modelling taken in this paper is somewhat different from that of conventional hydrologic simulation, and as such, requires a brief explanation. Conventional models of hydrologic systems consist of equations which propagate variables of interest forward through time. If observations of these variables are available, the difference between the observed and propagated values is taken to be the error of the model. There has been some recent work to use the difference in observed and simulated outflows to alter inflows to the system so as to reduce the error of the simulated outflows (Sittner and Krouse, 1979). All the models regard the error as the difference between observed and simulated values, and view the objective of the modeler as error reduction.

When optimal estimation is joined to hydrologic simulation, a different viewpoint must be taken. Each variable of interest is viewed as having three values associated with it at any time. First is the measurement of the variable. In the case of the reservoir model this is, for example, the measurement of the outflow. Second is the simulated value; i.e., the outflow predicted by the model equations. And third is the true value of the variable, a value which can never be known, but which modellers strive to estimate. The measured and simulated values are only approximations of the true value, and the information in each must be combined to obtain a better estimate of the unknown true value. The object of filtering theory is to obtain the best (i.e., minimum variance) estimate of the true value of a variable, given the model and measurement estimates of that variable.

In addition, optimal estimation theory treats the variables not simply as deterministic values, but instead as random variables which can be described by their probability density functions. The probability density function (pdf) of the best estimate of the true value is propagated through time. In general, this becomes an infinite dimensional problem which reduces its applicability in the estimation of real systems. To remove the intractability of infinite dimensional systems, only the first two moments of the pdf are considered. If an assumption of a Gaussian pdf is made, the pdf is completely described by its first two moments (mean and variance).

The solution to the optimal estimation problem is not known, in general, for nonlinear simulation models (Jazwinski 1970). For linear simulation models, an algorithm developed by Kalman optimally solves for the first two moments of the Gaussian pdf of the estimates of the true values of the variables of interest (Kalman 1960, Kalman and Bucy 1961). Documentation of this algorithm is extensive (Jazwinski 1970, Bras and Rodrigues-Iturbe 1972, Hino 1970, Moore 1971, Kitanidis 1978, Johnson and Bras 1978, Chiu 1978).

In general, the Kalman filter operates as a recursive predictor/corrector model. A summary of the Kalman filter algorithm is included in Appendix A. A system model is used to predict the mean and variance of the best estimate of the true value. When measurements are available, they are processed to correct the estimates based on this new information. The amount of correction is based on the relative uncertainty (variance) of the predicted estimate and the measurement. The technique is Bayesian with the a posteriori estimate following from the a priori estimate and the measurements.

CURRENT WORK

In this paper, a reservoir model is adapted to a Kalman filter configuration. The variables to be estimated are the inflow, outflow, and reservoir storage. The linear reservoir case is derived first. The inflow is modelled as a first-order autoregressive (AR) process (Fiering and Jackson 1971).

$$I_{t+1} = \rho I_t + (1-\rho)\,\bar{I} + \sigma_I\,(1-\rho^2)^{1/2}\,\omega_{It} \tag{3}$$

where ρ = the first order AR coefficient,

$\bar{I}$ = the average inflow,

σ_I = the standard deviation of the inflows, and

ω_{It} = a standard normal deviate.

The average outflow is a function of the storage during a time step.

$$\bar{Q}_{t+1} = k\,S_{t+1} \tag{4}$$

where

$$\bar{Q}_{t+1} = \frac{Q_{t+1} + Q_t}{2}$$

The change in storage over a time period is defined as the average inflow minus the average outflow.

$$\Delta S_{t+1} = S_{t+1} - S_t = \bar{I}_{t+1} - \bar{Q}_{t+1} \tag{5}$$

where

$$\bar{I}_{t+1} = \frac{R(I_{t+1} + I_t)}{2}$$

where R is the portion of inflow entering storage, and storage, inflow, and outflow all have units of volume. The coefficient R may be used to model losses, such as rainfall into infiltration.

Equation (3) propagates the inflow through time. The equations to model outflow and storage can be found from equations (3), (4), and (5) to be:

$$Q_{t+1} = \frac{Rk(1+\rho)}{(1+k)} I_t - Q_t + \frac{2k}{(1+k)} S_t + \frac{Rk(1-\rho)}{(1+k)} \bar{I} + \frac{Rk\sigma_I (1-\rho^2)^{1/2}}{(1+k)} \omega_{It} \qquad (6)$$

$$S_{t+1} = \frac{R(1+\rho)}{2(1+k)} I_t + \frac{1}{(1+k)} S_t + \frac{R(1-\rho)}{2(1+k)} \bar{I} + \frac{R\sigma_I(1-\rho^2)^{1/2}}{2(1+k)} \omega_{It} \qquad (7)$$

Equations (3), (6), and (7) can be written in matrix form as:

$$\hat{x}_{t+1} = F \hat{x}_t + D + G \omega_{It} \qquad (8)$$

where

$$\hat{x}_t = \begin{bmatrix} I_t \\ Q_t \\ S_t \end{bmatrix}$$

is the state vector at time t,

$$F = \begin{bmatrix} \rho & 0 & 0 \\ \frac{Rk(1+\rho)}{(1+k)} & -1 & \frac{2k}{(1+k)} \\ \frac{R(1+\rho)}{2(1+k)} & 0 & \frac{1}{(1+k)} \end{bmatrix}$$

is the state transition matrix,

$$D = \begin{bmatrix} 1 \\ \frac{Rk}{(1+k)} \\ \frac{R}{2(1+k)} \end{bmatrix} (1-\rho)\bar{I}$$

is the deterministic input vector,

$$G = \begin{bmatrix} 1 \\ \frac{Rk}{(1+k)} \\ \frac{R}{2(1+k)} \end{bmatrix} \sigma_I(1-\rho^2)^{1/2}$$

is the stochastic input vector.

Equation (8) is used in the predictive portion of the Kalman filter algorithm. The filter algorithm then uses available measurements to correct the predicted state vector, $\hat{x}_{t+1}$. The importance of measurements of one or more of the elements of the state vector is a function of the reduction in variance of the states because of the addition of those measurements. This can be seen in the following example.

Inflow, outflow, and storage data for a hypothetical reservoir were generated using equation (8) with a random number generator producing values of ω_{It}. These were considered as the true values (unknown in all real world cases) for a hypothetical reservoir. These true values were corrupted by the addition of a random error with zero mean and known standard deviation.

$$I^{o}_{t+1} = I_{t+1} + s_I \, \omega_{1t} \tag{9a}$$

$$Q^{o}_{t+1} = Q_{t+1} + s_Q \, \omega_{2t} \tag{9b}$$

$$S^{o}_{t+1} = S_{t+1} + s_S \, \omega_{3t} \tag{9c}$$

where the superscript o indicates observed; s_I, s_Q, and s_S are the standard deviations of measurement of inflow, outflow, and storage, respectively: and ω_{1t}, ω_{2t}, and ω_{3t} are standard normal deviates.

The procedure generated noisy data for a reservoir with known parameters. These data and the parameters for the hypothetical reservoir are shown in tables 1 and 2. The Kalman filter algorithm was run for eight cases that differed only in which combinations of variables were provided to the filter as observations. The results, indicating the importance of each observed variable, are shown in table 3. Not unexpectedly, the variance of all variables is smallest when measurements of all are provided, and largest when measurements of none are provided. To see which measurements improve the model performance, consider the states one at a time. Table 4 ranks the combinations of measured variables in the order of increasing variance for each state variable. If one could afford to obtain measurements of only two variables, the pair chosen would vary depending on which state variable was most important. It is interesting to note, however, that the pair would never be inflow and outflow measurements, which occur most commonly in conventional modelling.

Note, also, that for the state variables inflow and outflow, the pair of measurements chosen consists of the variable itself and the remaining variable with the smaller variance (i.e., the most additional information). For storage however, the measurement chosen besides that of the storage itself is the inflow, which has a higher variance than the outflow for this combination of measurements. An explanation for this choice lies in the fact that the covariance between storage and outflow is so large that there is little additional information about the storage in a measurement of the outflow that is not already accounted for in the measurement of the storage itself. The filter algorithm accounts for covariances between all states and measurements when making the corrections and, therefore, can recognize the actual new information that is added by each measurement.

NONLINEAR RESERVOIR

The Kalman filter requires a linear predictive model. In order to accommodate the filter for estimating with a nonlinear reservoir system model, a linearization by Taylor series expansion about the current storage was derived. For the nonlinear reservoir, equation (4) must be rewritten as

$$\bar{Q}_{t+1} = k\, S_{t+1}^{\alpha} \tag{10}$$

where $\alpha \neq 1$, in general.

After performing a Taylor expansion using equations (3), (5), and (10), and discarding terms higher than the first order, the equations for the nonlinear reservoir model are:

$$Q_{t+1} = \frac{R\beta(1+\rho)}{(1+\beta)} I_t - Q_t + \frac{2\beta-2k(\alpha-1)S_t^{\alpha-1}}{(1+\beta)} S_t + \frac{R\beta(1-\rho)}{(1+\beta)} \bar{I} + \frac{R\beta\sigma_I(1-\rho^2)^{1/2}}{(1+\beta)} \omega_{It} \tag{11}$$

$$S_{t+1} = \frac{R(1+\rho)}{2(1+\beta)} I_t + \frac{1+k(\alpha-1)S_t^{\alpha-1}}{(1+\beta)} S_t + \frac{R(1-\rho)}{2(1+\beta)} \bar{I} + \frac{R\sigma_I(1-\rho^2)^{1/2}}{2(1+\beta)} \omega_{It} \tag{12}$$

where $\beta = \alpha\, k\, S_t^{\alpha-1}$

and I_{t+1} is defined by equation (3).

Again, equations (3), (11), and (12) can be written in matrix form as:

$$\hat{x}_{t+1} = F_t \hat{x}_t + D_t + G_t\, \omega_{It} \tag{13}$$

where now:

$$F_t = \begin{bmatrix} \rho & 0 & 0 \\ \dfrac{R\beta(1+\rho)}{(1+\beta)} & -1 & \dfrac{2\beta-2k(\alpha-1)S_t^{\alpha-1}}{(1+\beta)} \\ \dfrac{R(1+\rho)}{2(1+\beta)} & 0 & \dfrac{1+k(\alpha-1)S_t^{\alpha-1}}{(1+\beta)} \end{bmatrix}$$

$$D_t = \begin{bmatrix} 1 \\ \frac{R\beta}{(1+\beta)} \\ \frac{R}{2(1+\beta)} \end{bmatrix} \quad (1-\rho)\bar{I}$$

$$G_t = \begin{bmatrix} 1 \\ \frac{R\beta}{(1+\beta)} \\ \frac{R}{2(1+\beta)} \end{bmatrix} \quad \sigma_I(1-\rho^2)^{1/2}$$

Note that now F_t, D_t, and G_t are functions of the current storage and will vary over time. Note also that equation (13) reduces to equation (8) if $\alpha = 1$, so the nonlinear case subsumes the linear case for reservoir models.

When $\alpha = 1$, the coefficient matrices F_t and G_t in equation (13) become time invariant. Since the quadratic forms of F_t and G_t are used in the filter variance equations, when F and G do not vary with time (and assuming a constant measurement error), the variance of the state variables will approach a steady-state value. For the general case of $\alpha \neq 1$, however, the variance of the state variables will be affected by the value of the current storage. These results can be seen in the following examples.

EXAMPLES

The improvement in modelling afforded by the union of reservoir models and filtering theory is demonstrated in the following examples. Data for the hypothetical reservoir described earlier were generated with the parameters shown in table 1.

The results of a simulation over 20 time periods are shown in figures 1, 2, and 3. The notation in figures 1 through 12 follows a common pattern. The solid line denotes the predicted values of either the mean or standard deviation of one of the state variables (inflow, outflow, or storage). The dashed line denotes the mean or standard deviation of observed values. The dotted line locates the mean or standard deviation of values corrected by the filter.

Note that the variance of the best estimate is less than the variance of either the observed or predicted values. Note, also, that the variance of the filtered estimate reduces over time to a steady state value. The filter improves its estimate as more data are processed until a saturation of data occurs. Improvement of the filtered estimate can be seen to produce improvement in the variance of the predicted value of the outflow, as the reservoir model starts predicting from a more certain position.

Data were also generated for a hypothetical reservoir identical to the above example, except that $\alpha = 5/3$. Results with notations similar to those above can be seen in figures 4, 5, and 6. Notice that the variance of the predicted values of outflow and storage vary with the storage volume.

A comparison of figures 1 and 4 shows that the means and variances for the inflow to the hypothetical reservoirs are slightly different for the cases of $\alpha = 1$ and $\alpha = 5/3$. This may seem surprising at first, because the inflow equation (3) does not depend on α, and the same sequence of standard normal deviates is used in both cases. The differences occur because as the Kalman filter algorithm corrects the states, all interactions among the state variables are accounted for. For example, if the observation of the storage and outflow indicate that less water should be in the reservoir than was predicted, all three state variables will be adjusted to achieve a balance. The relative adjustment of each is governed by the variances and covariances of all the states. The governing equations (1) and (2) will be satisfied at all times.

The next example demonstrates the use of optimal estimation in reservoir modelling for inflow and outflow data from a "typical catchment" (Lawler 1964, pp. 25-35 to 25-37). Data on the reservoir storage were not available, but optimal estimates are still computed for the storage value each time step. These estimates use measurements of inflow and outflow, and the relationships among the three state variables expressed in equation (13) to correct the storage estimate.

Data of inflow and outflow were used to determine parameters for a reservoir model. The error of inflow measurements was taken to be 15% of the standard deviation of the inflows. The error of outflow measurements was taken as 10% of the standard deviation of the outflow. For this example, the parameters are:

$$k = 0.415$$

$$\rho = 0.993$$

$$\sigma_I = 228.\ (\text{cfsd})^2$$

$$\bar{I} = 414.\ \text{cfsd}$$

$$\alpha = 1.$$

$$s_I = 34.\ \text{cfsd}$$

$$s_Q = 21.\ \text{cfsd}$$

The results shown in figures 7, 8, and 9 again show the variance reduction of the estimates from predicted or observed values. Note in figure 8, that for the above assumptions, the predicted outflow was improved so much that its variance was less than the variance of the observed outflow after three data values were processed.

Finally, a reservoir model with $\alpha = 5/3$ was fitted to the data from Lawler. In this case, $k = 0.002$. Figures 10, 11, and 12 show results for these data.

The variance of the storage reaches a minimum value as the reservoir fills. It appears that as the information about this particular storm event becomes available to the filter, better estimates of the storage can be made. As the reservoir empties, the information is depleted and the variance of the storage increases.

CONCLUSIONS

The value of conceptual reservoir models can be increased by adapting them to an optimal estimation formulation. Estimation of the inflow, outflow, and storage is improved, and an objective measure of the certainty of the estimation is available.

Table 1. Parameters and Data
for Hypothetical Reservoir

Parameter	Value
k	0.2
ρ	0.5
$\bar{I}$	10.0 (ℓ^3)
σ_I	5.0 (ℓ^3)
s_I	1.0 (ℓ^3)
s_Q	0.25 (ℓ^3)
s_S	0.2 (ℓ^3)

Table 2
Data Corrupted by Random Error

Time Step	$\alpha = 1.0$			$\alpha = 5/3$	
	Inflow(ℓ^3)	Outflow(ℓ^3)	Storage(ℓ^3)	Outflow(ℓ^3)	Storage(ℓ^3)
1	2.88	9.27	47.5	6.67	9.3
2	15.69	10.09	47.8	11.97	10.0
3	2.33	9.01	48.4	7.45	10.4
4	9.94	9.10	46.7	8.95	9.5
5	17.59	10.90	50.0	14.00	11.4
6	13.56	11.42	54.5	14.37	12.8
7	15.45	11.98	57.5	14.74	13.0
8	5.67	11.19	57.4	10.34	11.9
9	12.15	11.35	55.8	11.32	10.9
10	9.93	10.62	55.3	9.89	10.8
11	14.71	11.50	56.2	12.81	11.4
12	9.74	11.29	56.9	11.08	11.6
13	8.17	10.72	55.2	9.51	10.7
14	16.65	11.56	56.5	13.59	11.5
15	17.54	12.51	60.7	15.54	13.2
16	11.43	11.84	62.1	12.24	12.4
17	8.45	11.86	59.4	9.69	11.1
18	10.52	11.35	56.3	9.46	10.0
19	12.75	11.75	56.2	11.91	10.7
20	8.08	10.87	55.3	9.07	10.6

Table 3. Reduction of Variance by Addition of Observed States

Variables Observed	Variance After 20 Time Steps		
	I	Q	S
I,Q,S	0.438	0.008	0.034
Q,S	1.499	0.014	0.037
I,S	0.489	0.073	0.035
I,Q	0.722	0.280	0.461
S	2.263	0.092	0.040
Q	3.220	0.057	0.747
I	0.950	0.161	2.047
None	24.819	5.272	125.170

Table 4. Ranking of Combinations of Observed Variables in Order of Increasing Variance for Each State Variable

Ranking	State Variable		
	I	Q	S
1 (Smallest variance)	I,Q,S	I,Q,S	I,Q,S
2	I,S	Q,S	I,S
3	I,Q	I,Q	Q,S
4	I	Q	S
5	Q,S	I,S	I,Q
6	S	S	Q
7	Q	I	I
8 (Largest variance)	None	None	None

Appendix A

Summary of Kalman filter algorithm (Jazwinski, 1970, pp. 269-270).

Given a dynamical system model:

$$\hat{x}_{k+1} = F(k+1,k)\ \hat{x}_k + G(k)\ \omega_{k+1}$$

$$\hat{y}_k = H(k)\ \hat{x}_k + \nu_k$$

with $E(\omega_k) = 0$, $E(\omega_k\ \omega_\ell^t) = Q(k)\ \delta_{k\ell}$

$$E(\nu_k) = 0,\ E(\nu_k\ \nu_\ell^t) = R(k)\ \delta_{k\ell},\ R(k) > 0$$

Using the filter variables described in Table A.1, computations proceed as follows:

(1) Store the filter state
$\hat{x}(k|k)$, $\hat{P}(k|k)$;

(2) Predict the state
$\hat{x}(k+1|k) = F(k+1,k)\ \hat{x}(k|k)$;

(3) Compute the predicted error covariance matrix
$\hat{P}(k+1|k) = F(k+1,k)\ \hat{P}(k|k)\ F^t(k+1,k) + G(k)\ S(k+1)\ G^t(k)$
where superscript t indicates transpose;

(4) Compute the filter gain matrix
$C(k+1) = \hat{P}(k+1|k)\ H^t(k+1)\ [H(k+1)\ \hat{P}(k+1|k)\ H^t(k+1) + R(k+1)]^{-1}$
where superscript -1 indicates inverse;

(5) Process the observation y_{k+1}
$\hat{x}(k+1|k+1) = \hat{x}(k+1)|k) + C(k+1)\ [y_{k+1} - H(k+1)\ \hat{x}(k+1|k)]$;

(6) Compute the new error covariance matrix by
$\hat{P}(k+1)|k+1) = [I - C(k+1)\ H(k+1)]\ \hat{P}(k+1|k)$;
where I is the identity matrix;

(7) Set k = k+1, and return to step 1.

Table A.1 Filter Variables

Variable	Definition
$\hat{x}(k\|k)$	State estimate at t_k given $[y_1, y_2, \cdot\cdot, y_k]$
$\hat{P}(k\|k)$	Covariance matrix of the error in $\hat{x}(k\|k)$
$F(k+1,k)$	State transition matrix (from t_k to t_{k+1})
$G(k)$	System noise coefficient matrix
$S(k+1)$	System noise covariance matrix
$\hat{x}(k+1\|k)$	State estimate at t_{k+1} given $[y_1, y_2, \cdot\cdot, y_k]$
$\hat{P}(k+1\|k)$	Covariance matrix of the error in $\hat{x}(k+1\|k)$
$H(k+1)$	Measurement matrix
$R(k+1)$	Measurement noise covariance matrix
$C(k+1)$	Filter (Kalman) gain matrix at t_{k+1}
y_{k+1}	Measurement (observation) at t_{k+1}

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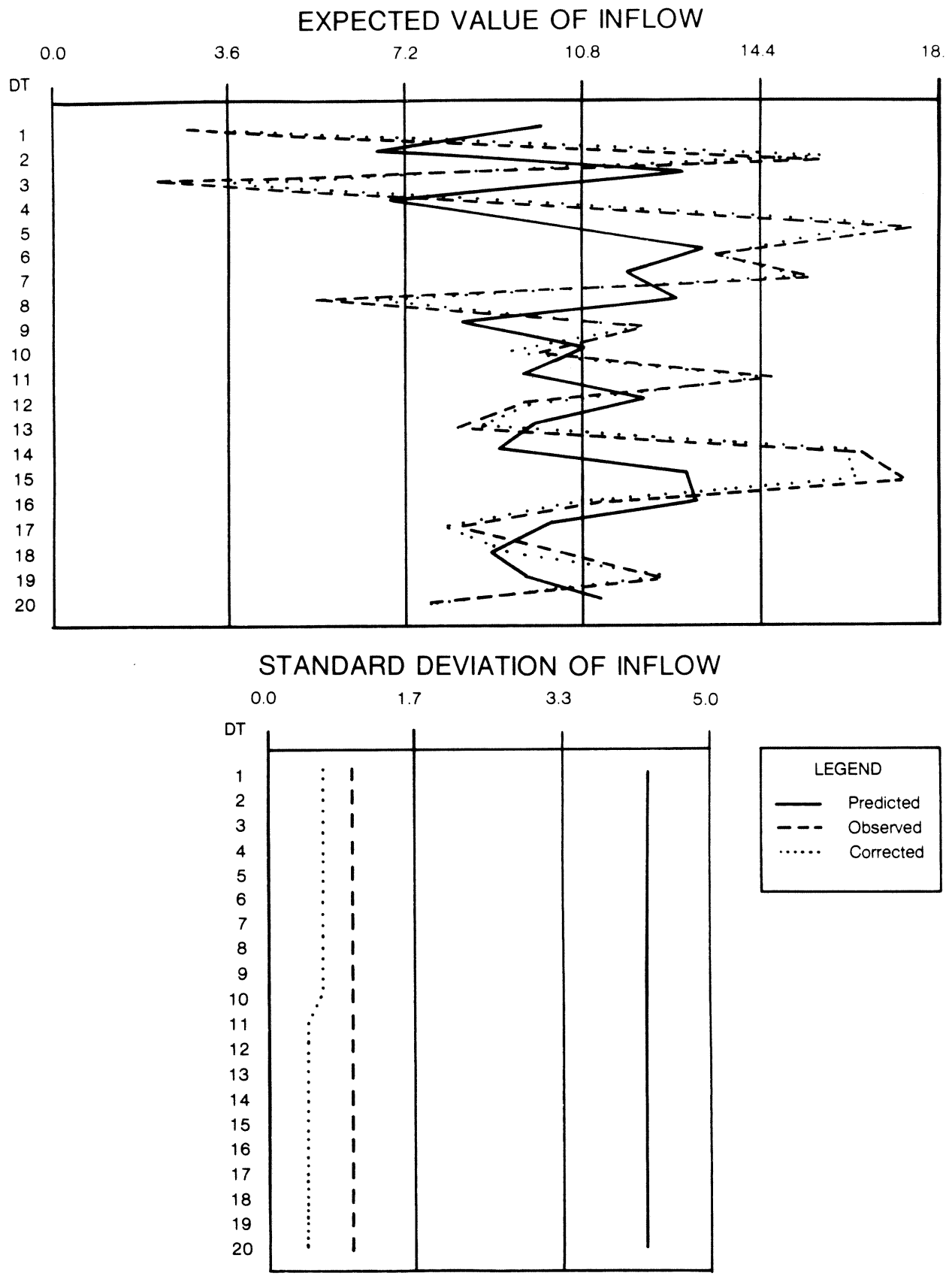

Figure 1: Inflow for Hypothetical Reservoir with $\alpha = 1$.

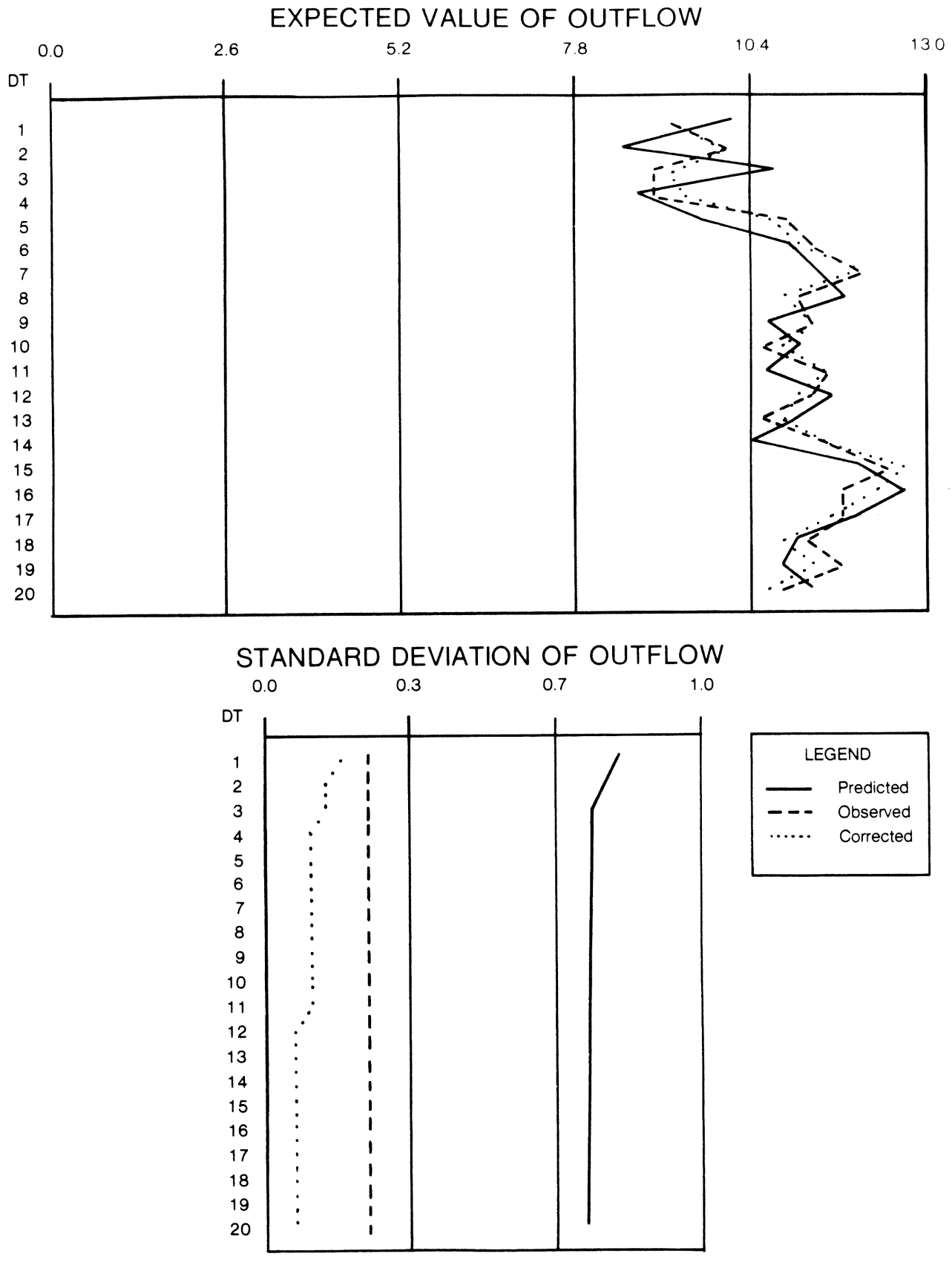

Figure 2: Outflow for Hypothetical Reservoir with $\alpha = 1$.

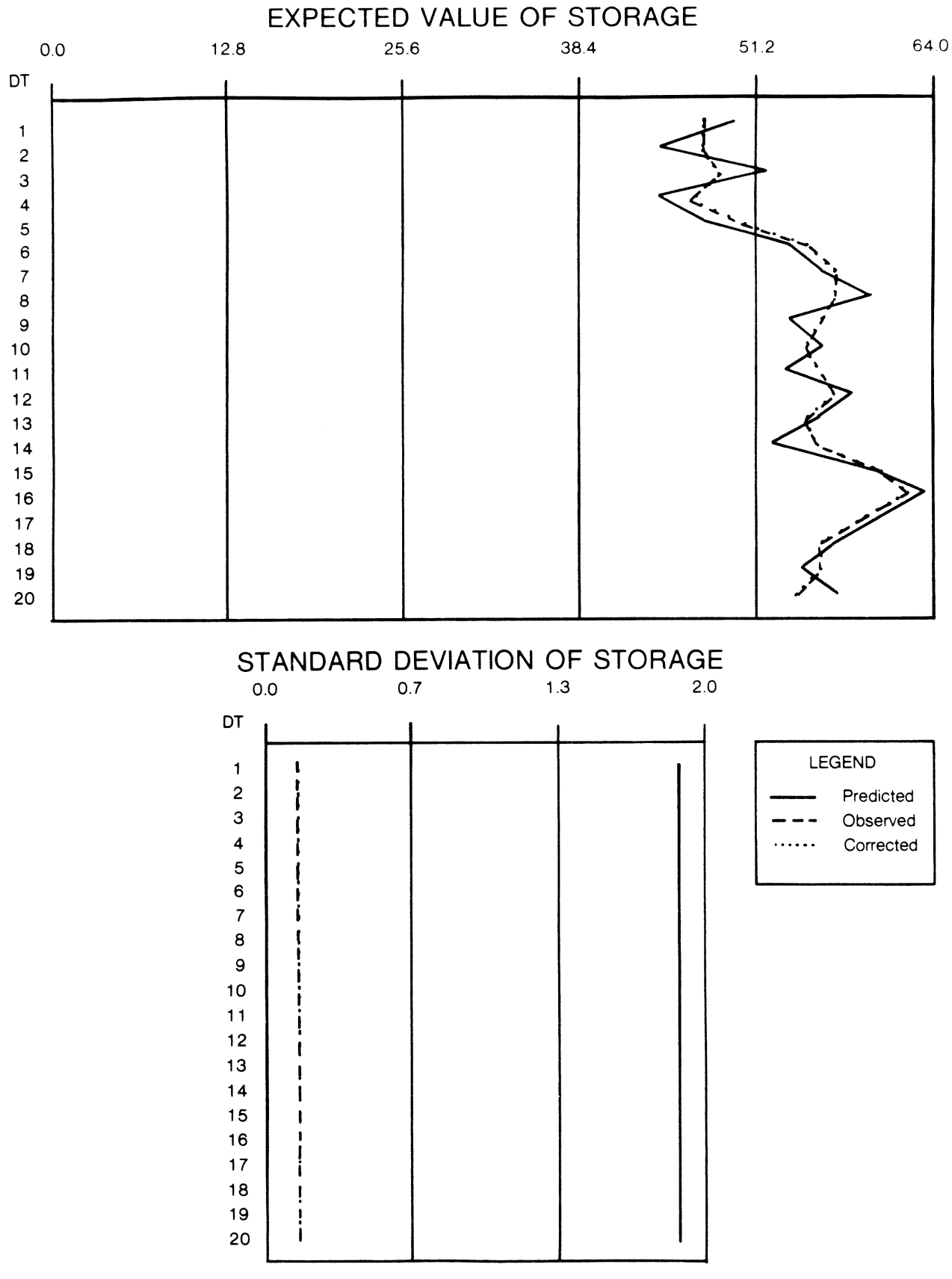

Figure 3: Storage for Hypothetical Reservoir with $\alpha = 1$.

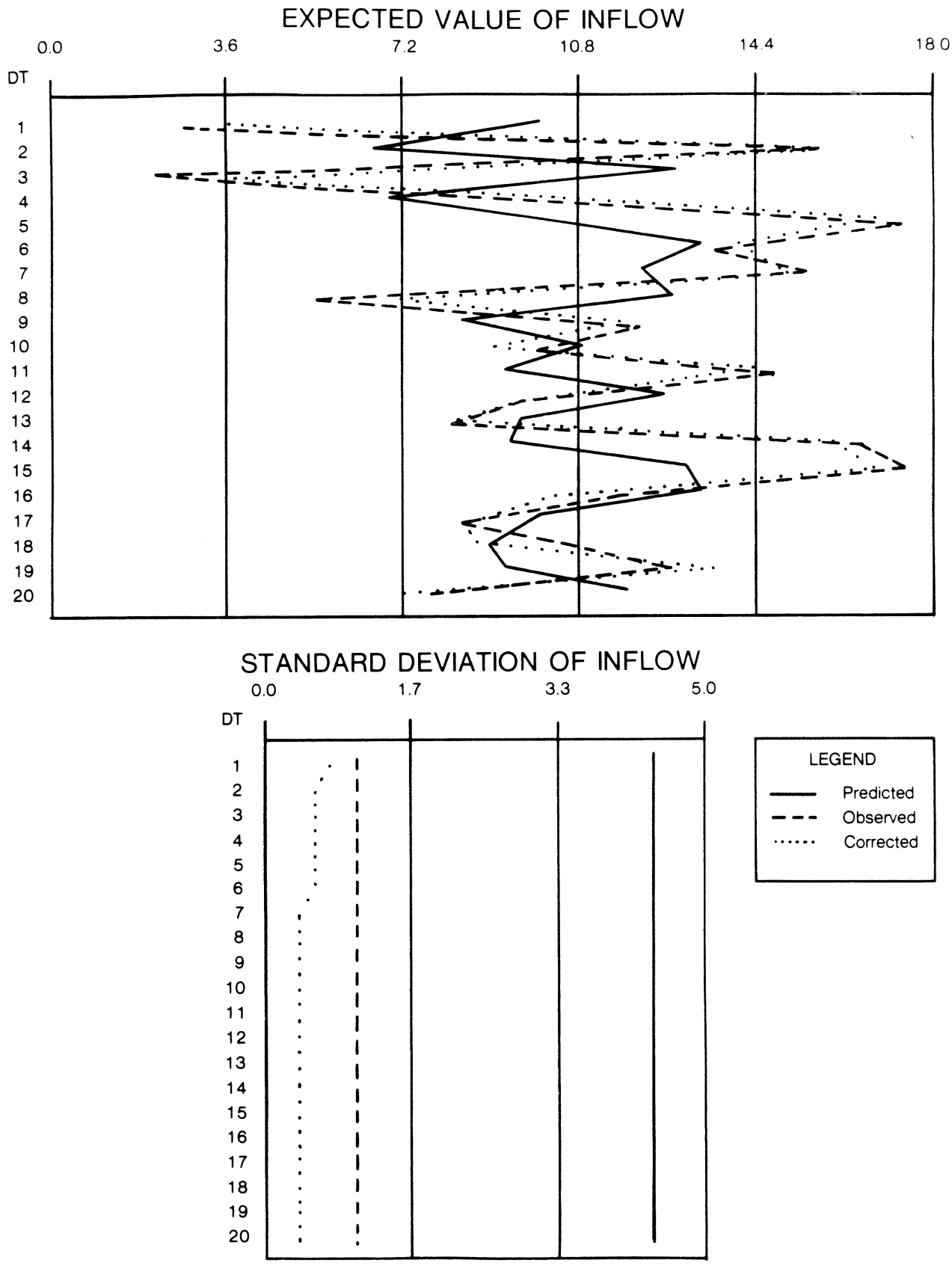

Figure 4: Inflow for Hypothetical Reservoir with $\alpha = 5/3$.

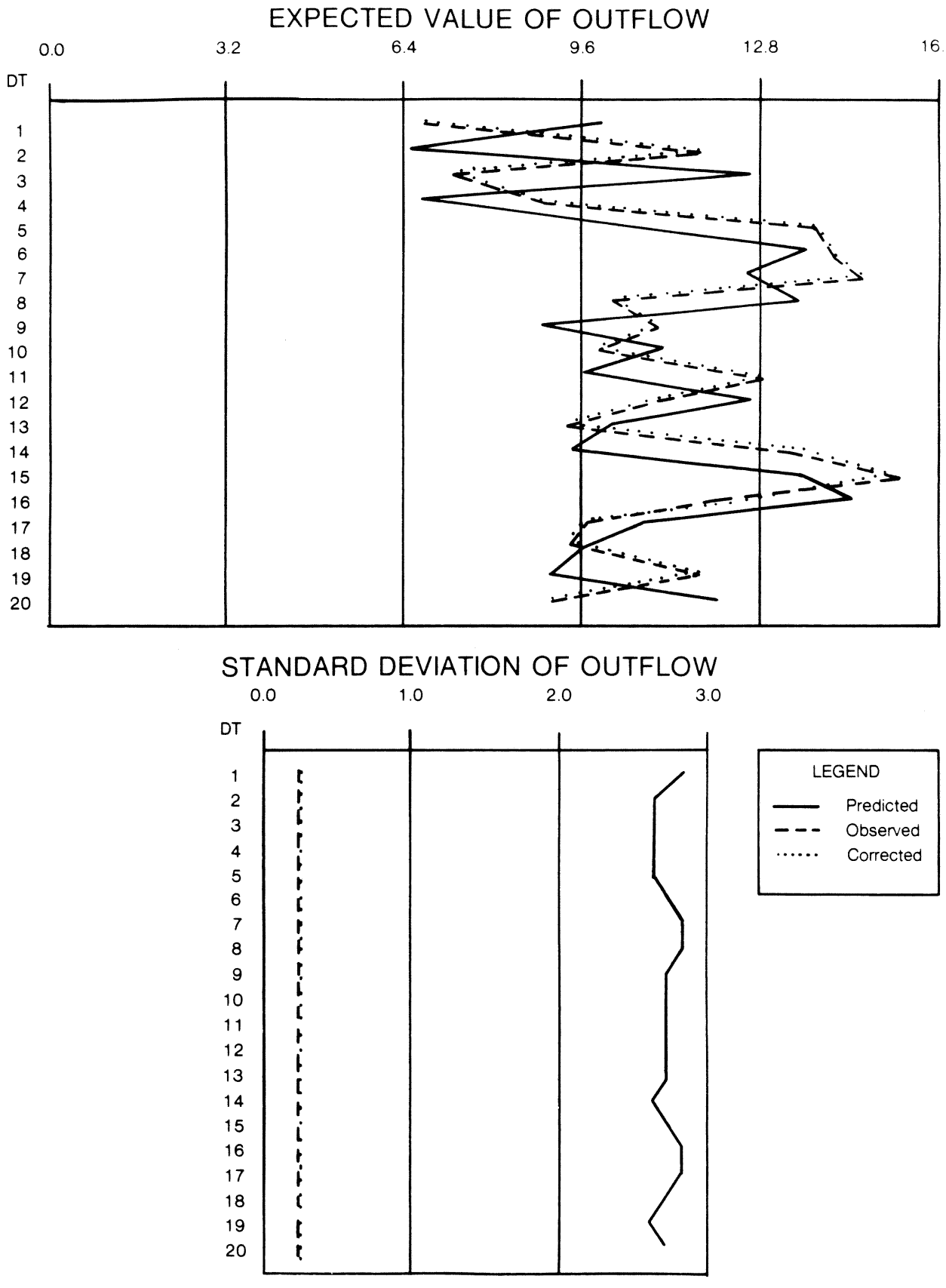

Figure 5: Outflow for Hypothetical Reservoir with $\alpha = 5/3$.

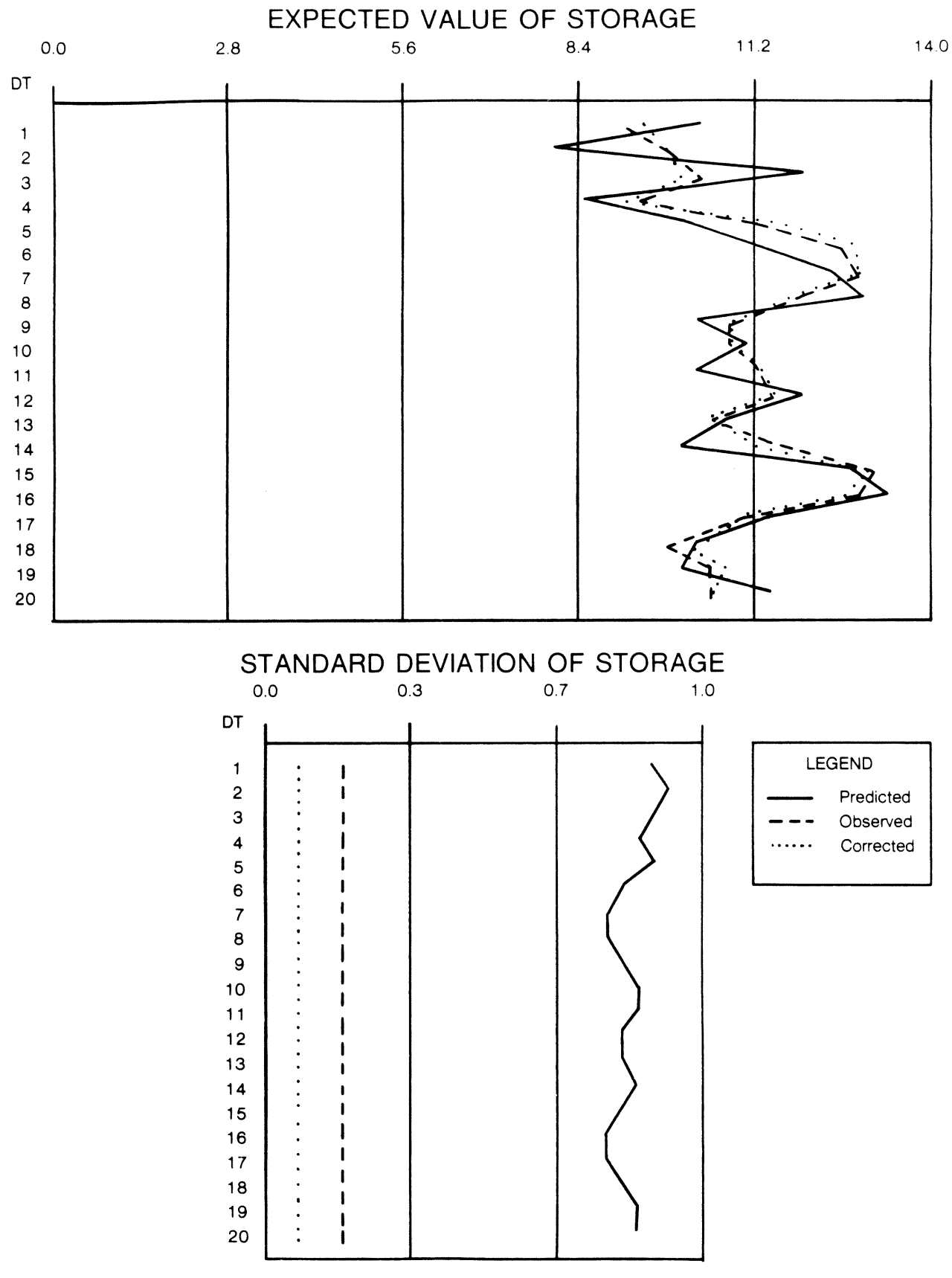

Figure 6: Storage for Hypothetical Reservoir with $\alpha = 5/3$.

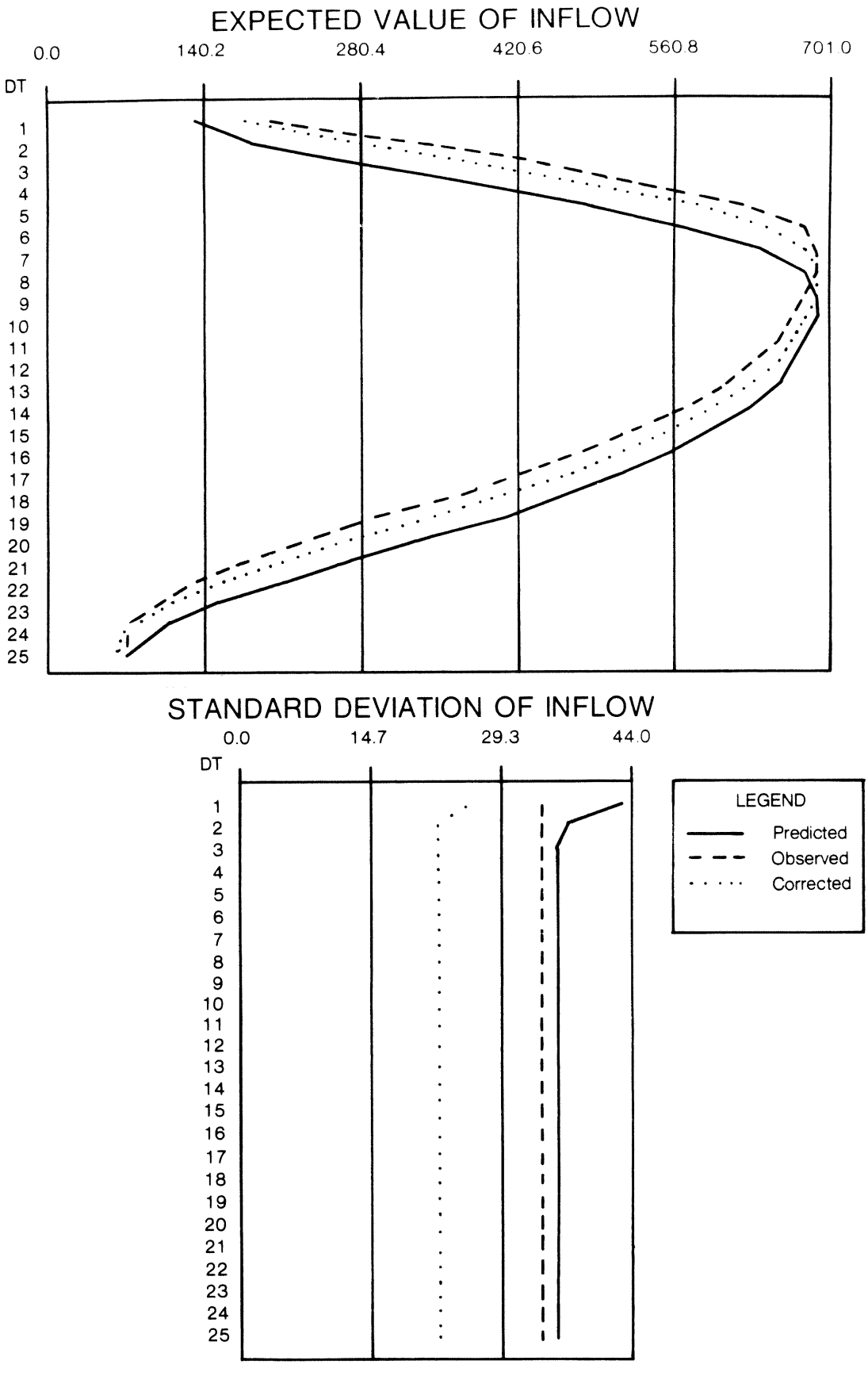

Figure 7: Inflow for Reservoir from Chow data with α = 1 and k = 0.415.

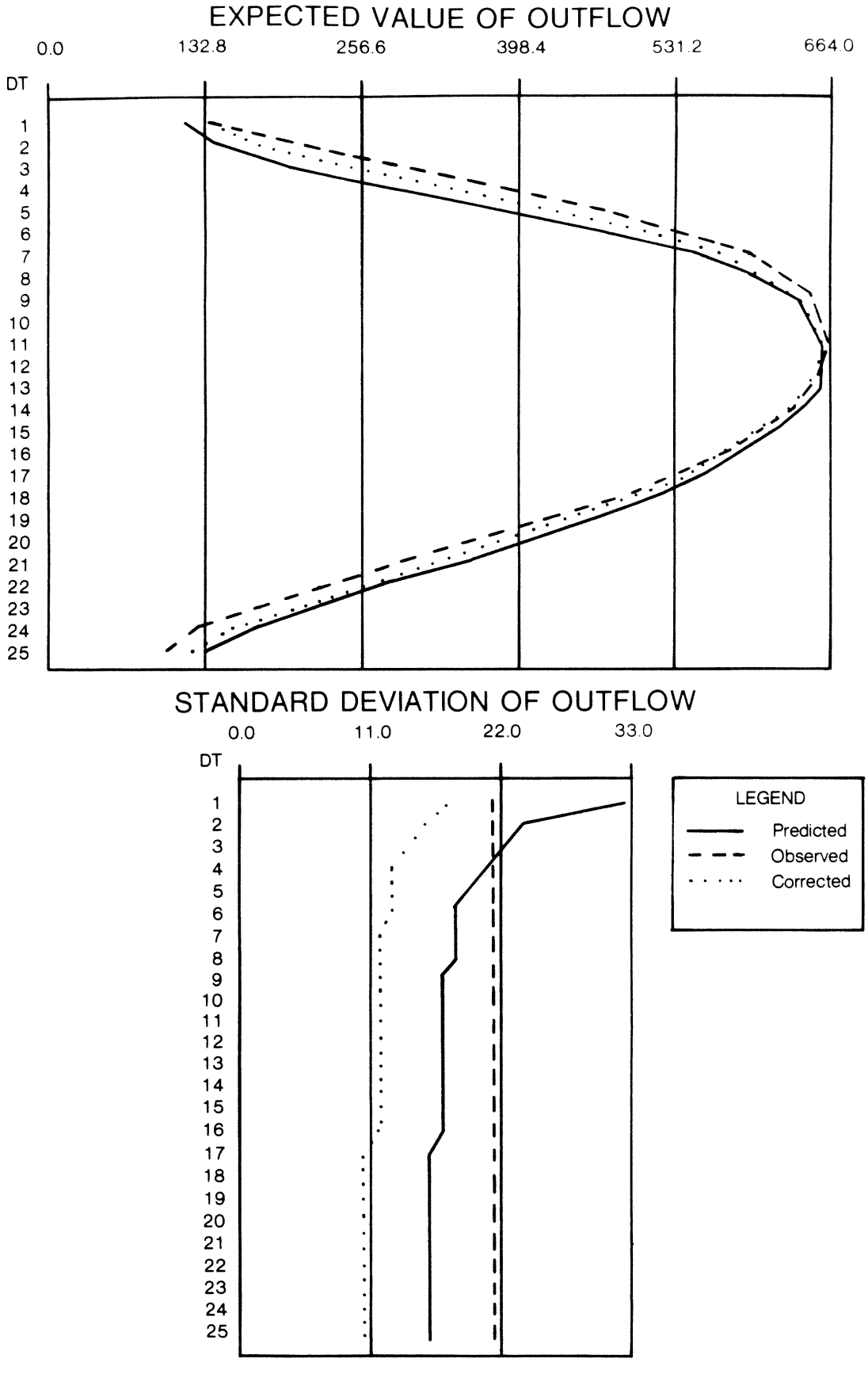

Figure 8: Outflow for Reservoir from Chow data with $\alpha = 1$ and k = 0.415.

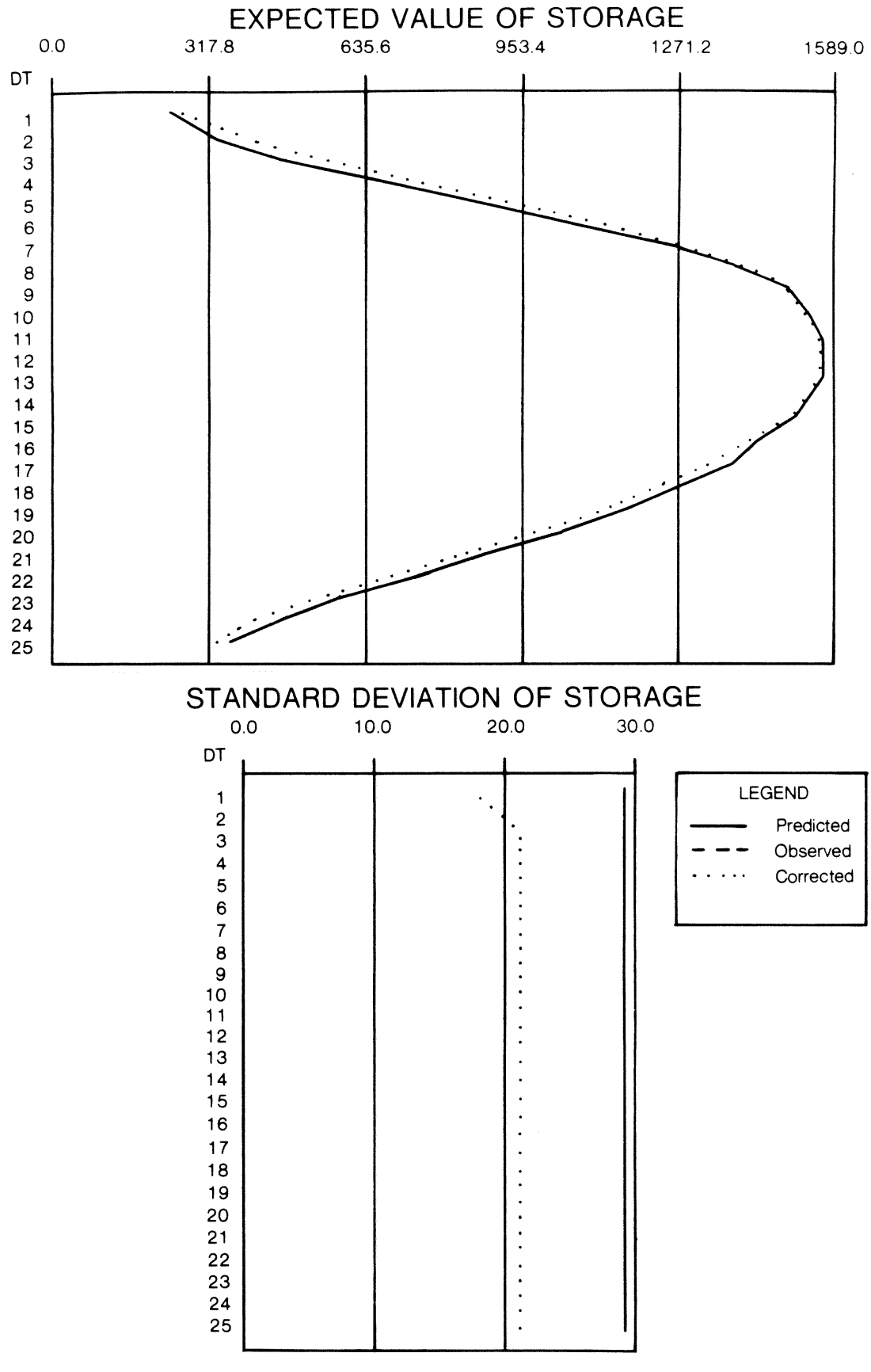

Figure 9: Storage for Reservoir from Chow data with $\alpha = 1$ and k = 0.415.

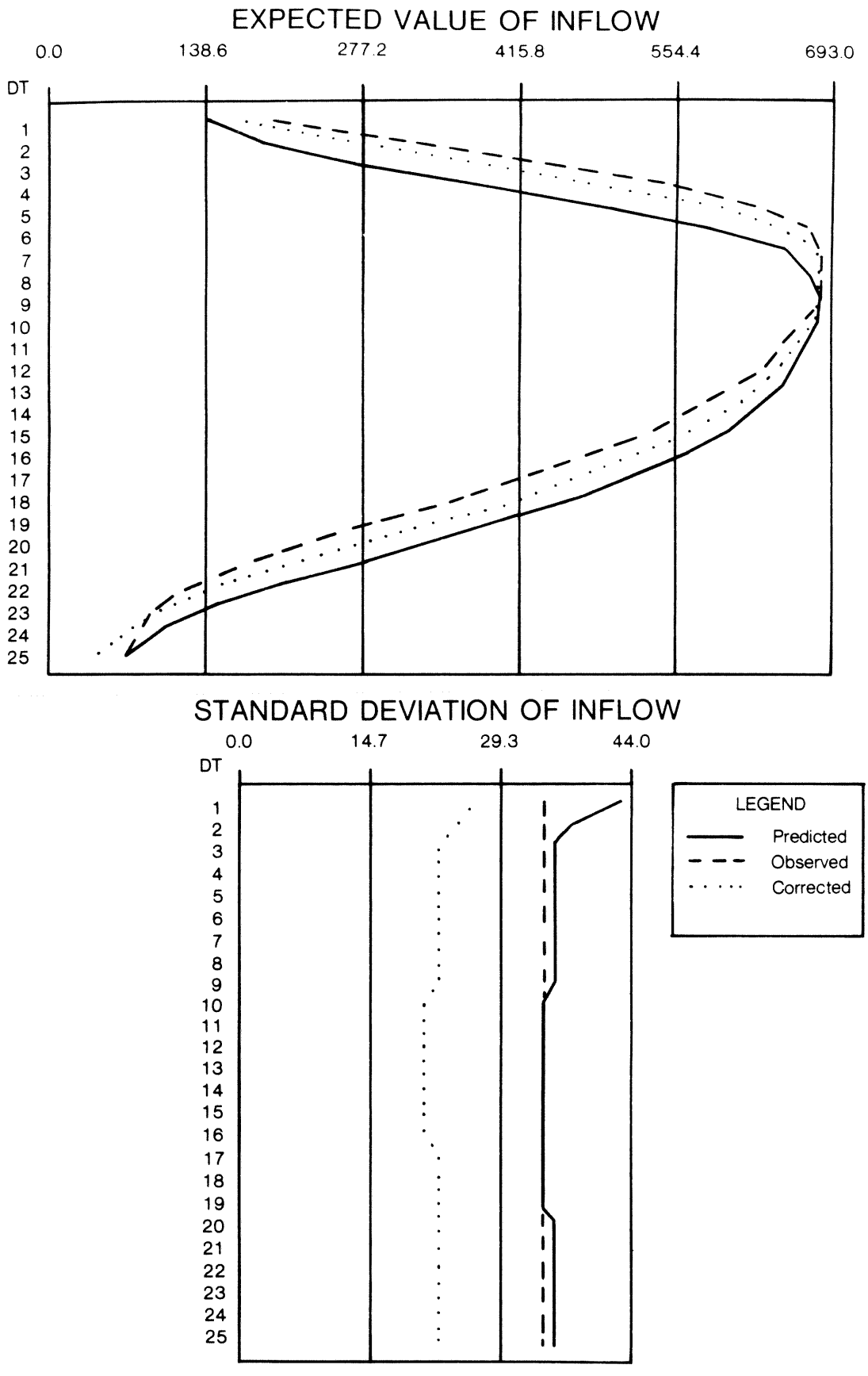

Figure 10: Inflow for Reservoir from Chow data with $\alpha = 5/3$ and k = 0.002.

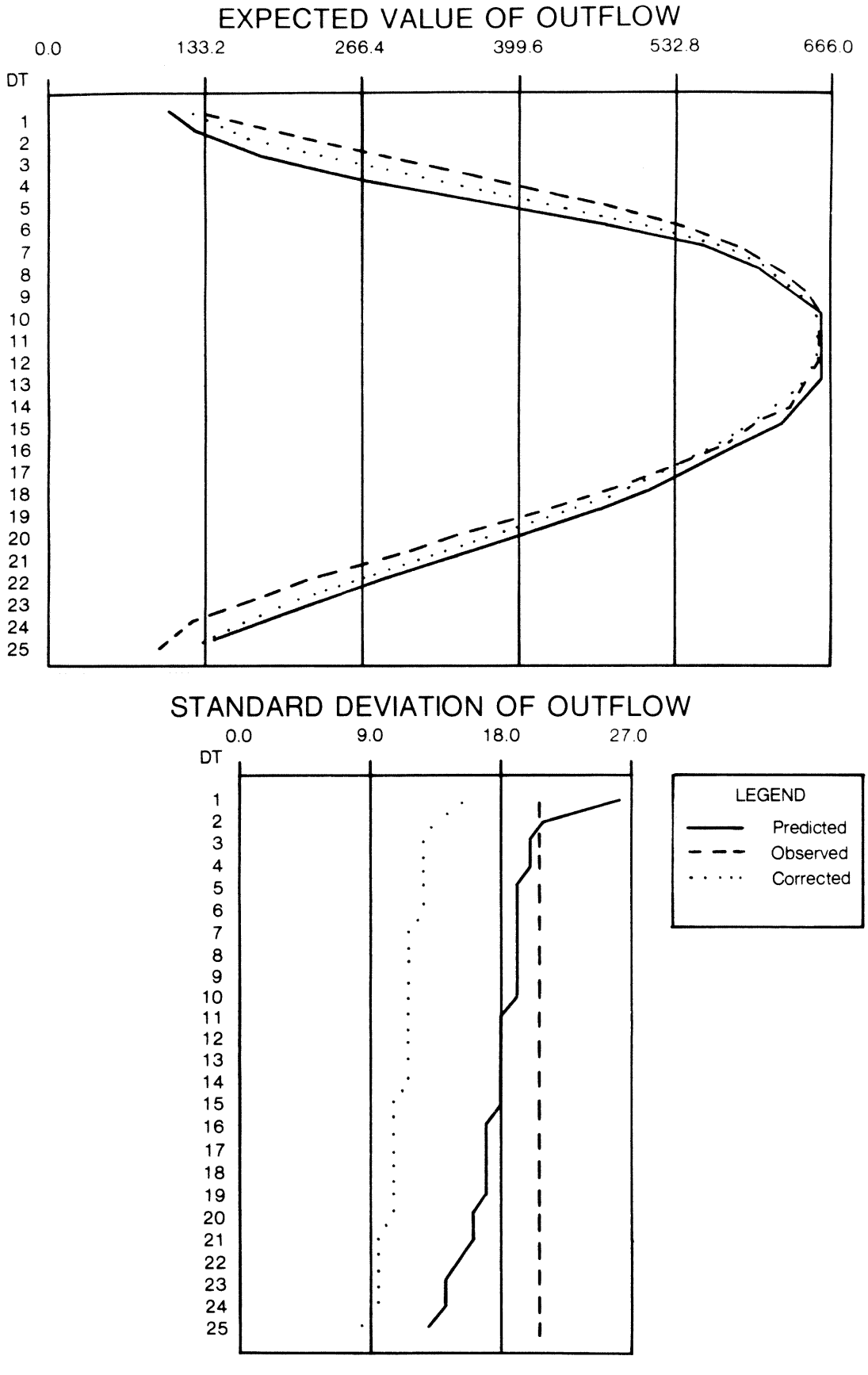

Figure 11: Outflow for Reservoir from Chow data with $\alpha = 5/3$ and k = 0.002.

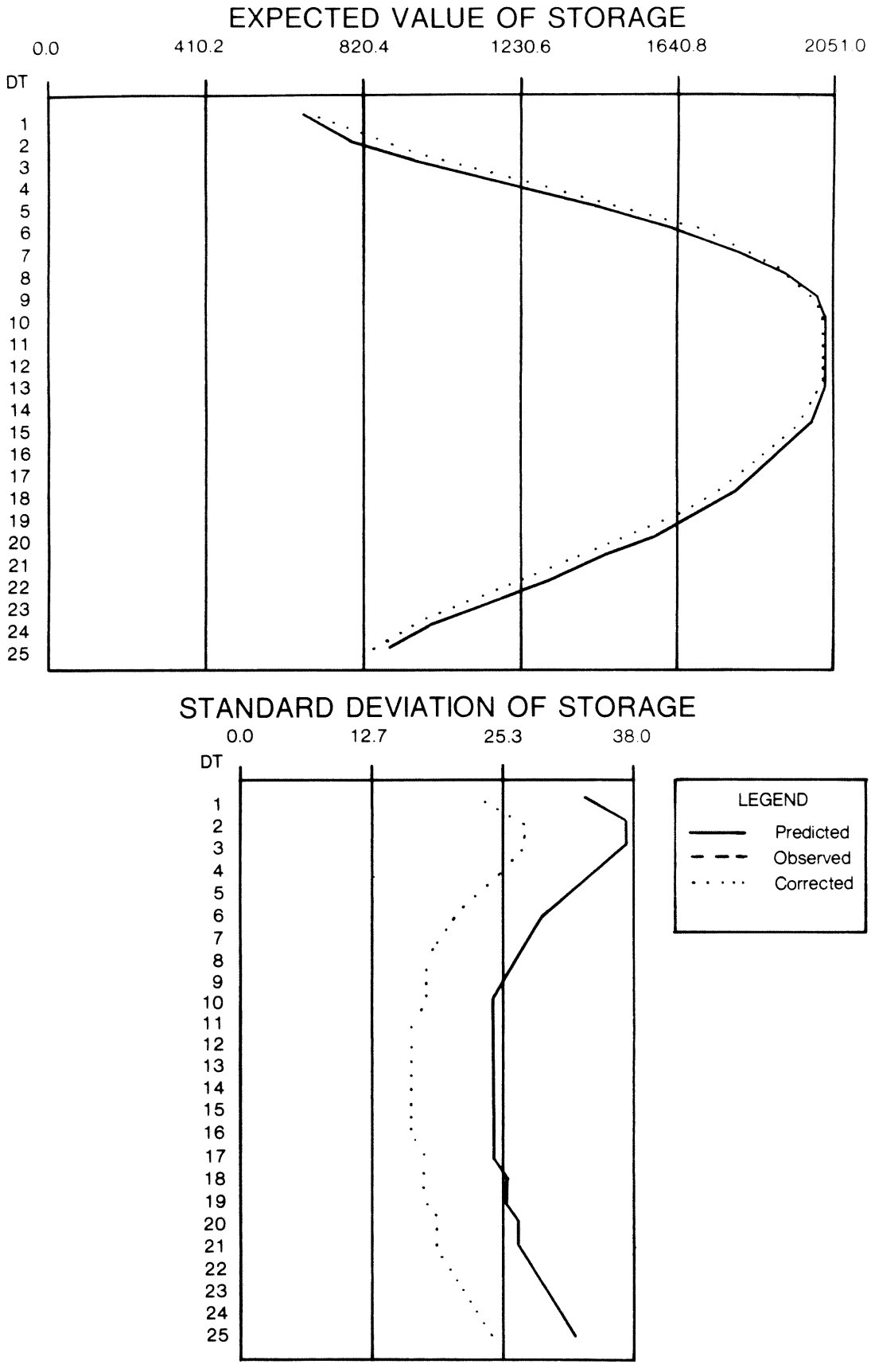

Figure 12: Storage for Reservoir from Chow data with $\alpha = 5/3$ and k = 0.002.