CHAPTER EIGHT

8. MODEL DEVELOPMENT: SIMPLIFIED COVARIANCE ESTIMATION

Development of the implicit soil moisture model ABDOMEN in Chapter 7 provided computational efficiency both in terms of forecasting the soil moisture states and forecasting of the soil moisture state covariances. However, the computation time for forecasting of the system state covariance matrix using the Kalman-filter in the three-dimensional field application (Chapter 11) was still very large. The reasons for this were: (i) evaluation of **A** (7.15) required inversion of Φ_1 and then multiplication by Φ_2 , resulting in a non-symmetric non-sparse matrix; and (ii) forecasting of the covariances required a triple matrix product with rather large (720 × 720) non-sparse, non-banded, non-symmetric matrices. Hence, this chapter develops a computationally efficient Modified Kalman-filter, which estimates the system state covariances by dynamics simplification, for updating of ABDOMEN3D in the three-dimensional field application presented in Chapter 11.

8.1 COVARIANCE ESTIMATION SCHEMES

System state covariance forecasting is widely recognised as being the most computationally expensive aspect of the Kalman-filter algorithm (Dee, 1991; Todling and Cohn, 1994; Dee, 1995). Computational requirements of the updating step of the Kalman-filter are less severe but non-trivial (Todling and Cohn, 1994), with forecasting of the system state covariances using the Kalman-filter (3.2) costing roughly 2N (where N is the number of system states) what it costs to produce the system state forecast (3.1) (Dee, 1991). While covariance forecasting is the central component of the Kalman-filter, implementation of the Kalman-filter as a scheme for data assimilation by "brute-force" is recognised as being unfeasible because of both its extensive computational requirements and a lack of complete knowledge of its required statistical inputs (Todling and Cohn, 1994).

Todling and Cohn (1994) noted that the lack of complete information concerning statistics of model errors, and even observation errors, makes the effort of evolving the complete forecast system state covariance matrix as dictated by the Kalman-filter not worthwhile. Furthermore, as a consequence of the assumptions in the Kalman-filter and the linearisation of state forecasting equations, even a full-fledged application of the extended Kalman-filter can do no better than to roughly approximate the actual forecast system state covariance evolution in an operational setting (Dee, 1991; Dee, 1995).

Accordingly, the covariance forecasting equation (3.2) is simply a means for representing the forecast system state covariances, which accounts in an approximate manner for the effects of error propagation by the forecast model (3.1) as well as for additional effects of model error. Hence, it follows that other approximations can be legitimately introduced in the extended Kalman-filter forecast system state covariance evolution, particularly in the computationally expensive propagation term (Dee, 1995).

A number of schemes for estimating the forecast system state covariance matrix have been presented in the literature and are reviewed by Todling and Cohn (1994). These simplified covariance estimation schemes have been divided into six main categories

- i) The *covariance modelling* category includes those schemes that assume a given form for the forecast system state covariance matrices, with no dynamics of these matrices taken into account.
- ii) *Dynamics simplification* encompasses those schemes using approximate but non-trivial system state dynamics to evolve the forecast system state covariances.
- iii) The *reduced resolution* approach decreases the dimensionality of the problem by computing the forecast system state covariances with a coarser resolution model than the model used to forecast the states. A hybrid of the dynamics simplification and reduced resolution schemes may also be considered.

- iv) *Local approximation* methods attempt to evolve the forecast system state covariance structure only for points separated by reasonably small distances.
- v) The *limiting filtering* approach computes a fixed gain matrix and an asymptotic system state covariance structure.
- vi) *Monte Carlo methods* attempt to estimate the forecast system state covariance matrix by integrating an ensemble of states between observation times.

In the Modified Kalman-filter developed in this chapter, the forecast system state covariances are estimated using the dynamics simplification approach.

8.2 COVARIANCE ESTIMATION BY DYNAMICS SIMPLIFICATION

An example of forecast system state covariance estimation by dynamics simplification is the Simplified Kalman-filter of Dee (1991). The basic idea behind the Simplified Kalman-filter is to predict the forecast system state covariance evolution by means of a simplified version of the forecast model itself, unlike the Kalman-filter, in which the full forecast model is used for error propagation. Moreover, the contribution to forecast system state covariance evolution due to model error forcing is approximated only as a final step at the end of the forecast cycle.

This thesis takes a slightly different tack for forecasting of the system state covariances. As the magnitude of variances in the forecast system state covariance matrix are controlled primarily by the system noise covariance matrix \mathbf{Q} (see section 3.3.2), which is generally poorly estimated, it is proposed to forecast only the correlations between system states. With an estimate of the correlation structure and an estimate of the forecast model system state variances (for instance, a standard deviation equal to 5% of the state value), the forecast system state covariance matrix can be easily assembled. This is termed the Modified Kalman-filter. If the essential aspects of the forecast system state dynamics can be captured by this simplified error model, the resulting loss of accuracy in estimating the forecast system state covariances should be acceptable, in view of

the many other approximations and lack of information associated with the Kalman-filter (Dee, 1995).

Forecasting of the system state covariance matrix with the original Kalman-filter is performed by $\mathbf{A}\Sigma\mathbf{A}^{T}$. Thus, the **A** matrix obviously contains information regarding the temporal (and spatial) evolution of the forecast system state covariance matrix. The **A** matrix itself is very noisy from one time step to the next, thus an auto-regressive smoothed value of **A** has been used to account for the smoothing effect of evaluating $\mathbf{A}\Sigma\mathbf{A}^{T}$.

Evaluating **A** at every time step using (7.15) is in itself computationally demanding, as a result of the matrix inverse and multiplication operations. Hence, a much more efficient way of obtaining an auto-regressive smoothed value of **A** is to evaluate auto-regressive smoothed values of Φ_1 and Φ_2 by

$$\overline{\Phi}_{1}^{n+1} = \alpha \overline{\Phi}_{1}^{n} + (1 - \alpha) \Phi_{1}^{n+1}$$
(8.1a)

$$\overline{\Phi}_2^{n+1} = \alpha \overline{\Phi}_2^n + (1 - \alpha) \Phi_2^{n+1}$$
(8.1b),

where $\overline{\Phi}$ is the auto-regressive smoothed value of Φ and α is a smoothing value close to 1. The auto-regressive smoothed value of **A** can then be evaluated when required by

$$\overline{\mathbf{A}} = \left[\overline{\Phi}_{1}\right]^{-1} \left[\overline{\Phi}_{2}\right] \tag{8.2},$$

where \overline{A} is the auto-regressive smoothed value of **A**. The correlation between states *i* and *j* are then estimated from

$$\Gamma = \overline{\mathbf{A}} \cdot \overline{\mathbf{A}}^{\mathrm{T}} \tag{8.3}$$

after reducing Γ to a correlation matrix (ie. 1 on the diagonal) by

$$\rho_{X_i,X_j} = \exp(\beta) \tag{8.4a},$$

where

$$\boldsymbol{\beta} = \left(1 - \frac{1}{\left(\Gamma_{i,j}\right)^a}\right) \cdot \boldsymbol{b} \tag{8.4b}$$

 $\Gamma_{i,j}$ is the *i,j*th element of Γ , while *a* and *b* are empirical coefficients. When $\Gamma_{i,j}$ is 1 then β equals 0 and the correlation is 1. Likewise, when $\Gamma_{i,j}$ is 0 then β equals $-\infty$ and the correlation is 0.

8.2.1 ESTIMATION OF EMPIRICAL COEFFICIENTS

In order to estimate the correlations between the system states using the dynamics simplification approach outlined above, it was necessary to evaluate appropriate values for the coefficients α , *a* and *b*. This was achieved by calibrating predicted correlations from the dynamics simplification procedure to the original Kalman-filter estimate of the correlations using NLFIT. This calibration was performed for a synthetic situation.

Using the soil parameters for a typical uniform clay (Soil Type 1) and initial soil moisture content (θ_i) given in Table 8.1, correlations between the nearsurface soil moisture state and deeper soil moisture states in a 1 m deep soil column were estimated. These correlations were estimated from the forecast system state covariance matrix from the original Kalman-filter with the simplified one-dimensional soil moisture forecasting model ABDOMEN1D. The soil moisture model was forced using a zero moisture flux boundary condition at the soil base and a 510 day extract of rainfall and evapotranspiration data collected at

Table 8.1: Soil parameters and initial soil moisture values for soil moisture profile simulation of Soil Type 1.

Layer	Thickness (mm)	θ, (%v/v)	K _s (mm/h)	φ (%v/v)	θ, (%v/v)	n	MGRAD
1	10	25	10.5	54	20	10.5	280
2	90	27					
3	200	29					
4	300	32					
5	400	35					



Figure 8.1: Comparison of the predicted (p) correlations (open symbols) using the dynamics simplification approach and the original Kalman-filter estimate of correlations (solid symbols) between the near-surface soil layer (1) and soil layers 2 to 5 for Soil Type 1 (ie. p1-4 is the predicted correlation between soil layers 1 and 4).

the Nerrigundah catchment, commencing from Julian day 130 1997 (Figure B.2 and Figure B.3 in Appendix B).

The coefficients α , *a* and *b* were calibrated as 0.995, 0.1 and 0.01 respectively, to yield the good comparison given in Figure 8.1. The value of α equal to 0.995 was chosen as a compromise between noise in the correlation estimate during periods of lower correlation, correct modelling of the overall shape of the time evolution of correlation, and correct estimation of correlation during periods of high correlation.

The soil moisture time series associated with the correlation time series in Figure 8.1 are given in Figure 8.2, where it can be seen that the correlation between the near-surface soil layer and the deeper soil layers was high when the soil profile was wet, and decreased as the soil profile dried. Moreover, this decrease in correlation with the near-surface layer as a function of soil moisture content increased with depth.

8.2.2 EVALUATION OF CORRELATION ESTIMATION PROCEDURE

The good fit obtained for the forecast correlations using the dynamics simplification with the original Kalman-filter estimate of correlations for Soil Type 1, may not hold for the previously calibrated values of the empirical coefficients (ie. $\alpha = 0.995$, a = 0.1 and b = 0.01), when the soil properties are altered. To investigate this, correlations were estimated using both the dynamics



Figure 8.2: Time series of simulated soil moisture content using Soil Type 1 for soil layer depths shown.

Layer	Thickness (mm)	θ _ι (%v/v)	K _s (mm/h)	φ (%v/v)	θ, (%v/v)	n	MGRAD
1	10	25	100	50	5	1.8	300
2	90	27	25	48	8	1.6	250
3	200	29	15	45	9	1.4	200
4	300	32	7	42	10	1.2	100
5	400	35	5	38	10	1.1	50

Table 8.2: Soil parameters and initial soil moisture values for soil moisture profile simulation of Soil Type 2.

simplification approach and the original Kalman-filter for two different soil types (Soil Types 2 and 3). Soil Type 2 has a varying soil texture, from a sandy loam through to clay (Table 8.2), while Soil Type 3 is a clay with uniform hydraulic conductivity, but varying soil porosity and residual soil moisture content (Table 8.3).

The correlation time series associated with Soil Types 2 and 3 are given in Figure 8.3 and Figure 8.4. The corresponding soil moisture time series show similar characteristics to those in Figure 8.2, and are consequently not shown. Figure 8.3 shows that the correlations from dynamics simplification are over-predicted relative to the original Kalman-filter estimate by as much as about 0.2 for Soil Type 2, while Figure 8.4 shows that the correlations from dynamics simplification are under-predicted relative to the original Kalman-filter estimate by only as much as about 0.05 for Soil Type 3 (neglecting the few spurious values).



Figure 8.3: Comparison of the predicted (p) correlations (open symbols) using the dynamics simplification approach and the original Kalman-filter estimate of correlations (solid symbols) between the near-surface soil layer (1) and soil layers 2 to 5 for Soil Type 2 (ie. p1-4 is the predicted correlation between soil layers 1 and 4).

Layer	Thickness (mm)	θ _ι (%v/v)	K _s (mm/h)	φ (%v/v)	θ, (%v/v)	n	MGRAD
1	10	25		54	5		
2	90	27		50	8		
3	200	29	10.5	45	10	1.8	280
4	300	32		42	12		
5	400	35		38	15		

Table 8.3: Soil parameters and initial soil moisture values for soil moisture profile simulation of Soil Type 3.

Given that the correlation between the near-surface soil layer and the deep soil layer during the dry period was so low (approximately 0.5) for Soil Type 2, the fact that the correlation was over-predicted by about 0.2 was not as important as it would be if the correlation was much closer to 1. The important point is, that the dynamics simplification approach developed in this chapter for estimating the correlations predicts the strong correlations very well, and at least qualitatively tracks the decrease in correlation during the drying periods. Moreover, the original Kalman-filter is itself only an estimate of the correlations, being dependent on the initial correlations specified and the linearisation of the forecasting model ABDOMEN1D. Hence a poor agreement between the correlations from the dynamics simplification approach and the original Kalmanfilter does not necessarily mean that correlations estimated from dynamics simplification approach are poor, only that it is a poor approximation of the Kalman-filter and its assumptions.



Figure 8.4: Comparison of the predicted (p) correlations (open symbols) using the dynamics simplification approach and the original Kalman-filter estimate of correlations (solid symbols) between the near-surface soil layer (1) and soil layers 2 to 5 for Soil Type 3 (ie. p1-4 is the predicted correlation between soil layers 1 and 4).

While the dynamics simplification approach for approximating the correlation between soil layers appeared adequate for a one-dimensional soil column using ABDOMEN1D, its applicability to estimating the spatial correlations from the three-dimensional soil moisture forecasting model ABDOMEN3D had not been verified. To verify that correlations resulting from the lateral redistribution of soil moisture content, in addition to those from the vertical redistribution of soil moisture content, were correctly identified, a comparison of correlations from the dynamics simplification approach and the original Kalman-filter was made (Figure 8.5). Due to the computational constraints of the original Kalman-filter, this comparison was made for a twodimensional planar hillslope having uniform soil thickness and slope, using ABDOMEN3D. The hypothetical planar hillslope catchment consisted of an 180 m long hillslope of 1% slope, with a 20 m grid resolution. The soil profile was 1 m deep and had the soil parameters of Soil Type 2. Soil Type 2 parameters were used, as these gave the worst comparison between the correlation forecasts from the dynamics simplification approach and the original Kalman-filter, for the one-dimensional soil profile. The system states and corresponding correlations were forecast for the planar hillslope by subjecting the forecasting model ABDOMEN3D to the same boundary conditions as for the one-dimensional simulations.

Figure 8.5 shows a poor comparison between the forecasts of lateral correlations using the dynamics simplification approach and the original Kalmanfilter. However, correlation forecasts from the dynamics simplification approach compared well with correlation estimates from an analysis of the simulated soil moisture contents. This suggested that the proposed method for estimating correlations from ABDOMEN3D was adequate. Furthermore, the forecast correlations from dynamics simplification agreed with intuition, showing both a decrease in correlation with depth in the soil profile and separation from the reference grid element.

As mentioned in the previous discussion of correlation forecasts using the one-dimensional model, poor comparisons between the correlation forecasts using the original Kalman-filter and the dynamics simplification approach only means that the dynamics simplification approach is a poor representation of the original Kalman-filter and its assumptions. It does not mean that the correlation forecasts using the dynamics simplification approach are incorrect. The poor comparison of correlation forecasts from the dynamics simplification approach with those from the original Kalman-filter are, in addition to errors in covariance forecasting from model linearisation and the application of model noise, a result of the original Kalman-filter state covariance matrix initialisation.

In the above simulation, the initial system state covariance matrix for system state covariance forecasting by the original Kalman-filter was initialised with zero correlation between all layers and grid cells. Forecasting of system state covariances with the original Kalman-filter was not as strong between grid cells as it was between the layers of a grid element, as the lateral redistribution of soil moisture was less dominant than the vertical redistribution. This was due to the low slope angle and the application of an isotropic hydraulic conductivity in the system state forecasting model. If the slope angle was greater and/or there was a non-isotropic hydraulic conductivity, with hydraulic conductivities being greater for the lateral direction than for the vertical direction, then the situation would be different.

As a result of the soil moisture dynamics in these simulations being dominated by the vertical redistribution of soil moisture, forecasts of system state covariances using the original Kalman-filter were heavily influenced by the system state covariance matrix initialisation. This indicates that initialisation of the system state covariance matrix would be an important task for updating of the forecast with the original Kalman-filter when using ABDOMEN3D. However, initialisation of the system state covariance matrix for one-dimensional simulations using ABDOMEN1D was relatively unimportant, as a result of the stronger dependence of soil moisture at short length scales.

8.3 EVALUATION OF THE MODIFIED KALMAN-FILTER

It has been shown in the previous section that the prediction of correlations using the dynamics simplification approach and specification of a standard deviation to construct the forecast system state covariance matrix (Modified



Figure 8.5: Comparison of the predicted (p) correlations (open symbols) using the dynamics simplification approach and the original Kalman-filter estimate of correlations (solid symbols) between the near-surface soil layer (1) of uphill grid cell (1) for Soil Type 2, against layers of: a) grid cell 2; b) grid cell 3; c) grid cell 4; and d) grid cell 5 (ie. p11-54 is the predicted correlation between grid cell 1 layer 1 and grid cell 5 layer 4 using dynamics simplification).



Figure 8.5 (con't): Comparison of the predicted (p) correlations (open symbols) using the dynamics simplification approach and the original Kalman-filter estimate of correlations (solid symbols) between the near-surface soil layer (1) of uphill grid cell (1) for Soil Type 2, against layers of: e) grid element 6; f) grid element 7; g) grid element 8; and h) grid element 9 (ie. p11-83 is the predicted correlation between grid cell 1 layer 1 and grid cell 8 layer 3 using dynamics simplification).

Kalman-filter) resulted in a somewhat different covariance matrix than what the original Kalman-filter would forecast. However, the important issue is the ability to make improvements to the forecasting of soil moisture profiles using the Modified Kalman-filter. To evaluate this, the Modified Kalman-filter was applied to a synthetic one-dimensional soil column with Soil Types 1, 2 and 3, and compared with "true", open loop and original Kalman-filter simulations.

The "true" soil moisture profiles are synthetic data generated from ABDOMEN1D, while the open loop refers to the situation where no observations were used to update the soil moisture model. Synthetic data has been used, so that the Modified Kalman-filter could be evaluated against the original Kalman-filter independent of the effects from model error on the retrieval of the "true" soil moisture profile. The Modified Kalman-filter was only evaluated for a one-dimensional soil column, due to the computational constraints of applying the original Kalman-filter to the spatially distributed problem and the stronger correlations between soil layers than between grid cells. Hence, the results from this investigation should be indicative of those from application of the Modified Kalman-filter to the spatially distributed problem. Evaluation of the Modified Kalman-filter for the spatially distributed problem is left for the field application in Chapter 11.

The "true" soil moisture profiles were produced from simulations with ABDOMEN1D, subject to a zero flux boundary condition at the base of the 1 m deep soil column and surface forcing data collected at Nerrigundah from Julian day 130 1997 to Julian day 274 1998 (Figure B.2 and Figure B.3). This is same surface forcing data used in the earlier sections of this chapter. The initial soil moisture profile and soil parameters are given in Table 8.1 to Table 8.3. Open loop and soil moisture profile estimation simulations were initialised with a poor initial guess of the soil moisture profile of 50% v/v, 38% v/v and 38% v/v uniform throughout the soil profile, for Soil Types 1, 2 and 3 respectively.

The original Kalman-filter was initiated with a diagonal covariance matrix with zero correlation and 50% v/v standard deviations. The system noise covariance matrix had zero correlation and variances of 5% of the system state per half hour. The observations were taken from the "true" simulation of the top 1 cm

soil layer, with a standard deviation of 2% of the observation used for the observation noise. The Modified Kalman-filter used a forecast system state standard deviation of 5% of the system state value for estimating the forecast system state covariance matrix from the forecast correlations using the dynamics simplification approach.

The results from these simulations are given in Figure 8.6, Figure 8.7 and Figure 8.8 for Soil Types 1, 2 and 3 respectively. It can be seen from these simulations that retrieval of the "true" soil moisture profile occurred very quickly (within 10 days or 2 updates) for both the original and Modified Kalman-filter assimilation schemes in all three cases. Once the "true" soil moisture profile was retrieved, the soil moisture profile estimation algorithm continued to track the "true" soil moisture profile. This was expected as the same model and boundary conditions were used to generate the "true" soil moisture profiles as were used to estimate the soil moisture profile using the near-surface soil moisture observations.

The simulations also show that the open loop simulation came on track towards the end of the dry summer period for Soil Type 1, while the open loop simulation came on track during the first wetting up period for Soil Types 2 and 3. The reason why simulations for Soil Types 2 and 3 came on track so early was that they had a lower soil porosity and hence lower total soil moisture storage. Thus during the wetting up period, both "true" and open loop simulations went to saturation for Soil Types 2 and 3, while only the open loop simulation went to saturation for Soil Type 1. This suggests that providing the soil porosity and residual soil moisture content parameters are correctly identified in the soil moisture model, then model estimates of soil moisture content may be correct during very dry and very wet periods, without any assimilation. Moreover, it supports the idea of re-setting model simulations of soil moisture content under extreme conditions.

The soil moisture profile simulations presented above, have displayed a good comparison between soil moisture profile estimation results when using the Modified Kalman-filter and original Kalman-filter assimilation schemes. However, the "true" soil moisture profile was retrieved during early updates,



Figure 8.6: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 1, standard deviations were 5% of the state values.



Figure 8.7: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 2, standard deviations were 5% of the state values.



Figure 8.8: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 3, standard deviations were 5% of the state values.

where there was a good agreement between the correlation forecasts using both the dynamics simplification approach and the original Kalman-filter (see Figure 8.1, Figure 8.3 and Figure 8.4). As predictions of the correlation were comparatively poor during the dry summer period, the above simulations were repeated, starting from simulation day 250, with the Kalman-filter and open loop simulations initialised with the same poor initial guess as before. The significance of these simulations was to evaluate the Modified Kalman-filters ability to make improvements to the soil moisture profile estimate, when the forecast correlations differed most from those of the original Kalman-filter, and the initialisation of the soil moisture profile was poor. The results from these simulations are given in Figure 8.9, Figure 8.10 and Figure 8.11 for Soil Type 1, 2 and 3 respectively.

The simulation results have shown that both the original and Modified Kalman-filter simulations retrieved the "true" soil moisture profile after only 1 update for Soil Type 1. Apart from the deeper layers, the soil moisture profile estimation algorithm using both the original and Modified Kalman-filter assimilation schemes continued to track the "true" soil moisture profile exactly, with only a few percent discrepancy between the "true" and estimated soil moisture values from the Modified Kalman-filter at deeper depths. In comparison, the open loop profile did not align with the "true" soil moisture profile until both the "true" and open loop simulations reached saturation.

Soil Type 2 results were much poorer than Soil Type 1, both in terms of the ability to retrieve the soil moisture profile using the Modified Kalman-filter and its comparison with the original Kalman-filter simulations. Given the poorer comparison of forecast correlation using the dynamics simplification approach with that from the original Kalman-filter for Soil Type 2 (Figure 8.3), it is not surprising that there was a greater discrepancy between the Modified and original Kalman-filter simulations than for Soil Type 1.

Simulations of the soil moisture profile for Soil Type 2 have shown a poor estimation of the soil moisture content at deeper soil layers using both the Modified and original Kalman-filter assimilation schemes. While the near-surface soil layers came on track with the "true" soil moisture content after only 1 update, the deeper soil layers were over-corrected in the first update, and did not come on



Figure 8.9: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 1, standard deviations were 5% of the state values.



Figure 8.10: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 2, standard deviations were 5% of the state values.



Figure 8.11: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 3, standard deviations were 5% of state values.

track until the wetting up period. The reason for this was that soil moisture content in the observation layer followed the observed soil moisture content almost exactly, even though the soil moisture content of deeper soil layers was incorrect.

The reason why no improvement was made in the deeper soil layers when the soil moisture model accurately forecast the near-surface soil moisture content may be seen from the Kalman-filter update equation in (3.4). The Kalman-filter update equation adjusts the system state forecast by adding a correction term, which is the Kalman-filter gain multiplied by the difference between the observations and the system state forecast. The Kalman-filter gain is evaluated as a function of the observation and forecast system state covariance matrices. Hence, if there is no discrepancy between the forecast system states and the observations, then the Kalman-filter cannot make any adjustment to the state forecast of deeper depths, irrespective of the assumptions made in evaluating the observation and system state covariance matrices, and hence Kalman-filter gain.

The phenomenon of decoupling between the near-surface soil moisture content and that of deeper soil layers has been observed in the field by Capehart and Carlson (1997), as a result of divergence between the drying rates at the surface and deeper levels. The significance of this is that when the near-surface soil layer becomes decoupled from the deep soil layers, the near-surface soil layer does not reflect the soil moisture status of deeper soil layers. Hence, under decoupled conditions, there can be no updating of the soil moisture profile once the near-surface soil layer correctly tracks the near-surface soil moisture content. This decoupling is indicated in Figure 8.3 for simulations with Soil Type 2, by the low correlation between deeper soil layers and the near-surface soil layer.

This suggests that if a system update is performed too soon after initialisation of the forecasting model and the associated covariance matrix, then the Kalman-filter will update the near-surface soil layer correctly, but incorrectly for the deeper soil layers, as the forecast system state covariances are still affected by the initial conditions. If the near-surface layer and deep soil layers are decoupled, then estimation of the soil moisture profile will continue to be poor. Simulation results for Soil Type 3 have shown that retrieval of the "true" soil moisture profile occurred after the first update with the original Kalman-filter, while the Modified Kalman-filter over-corrected on the first update. The Modified Kalman-filter then oscillated around the "true" soil moisture at deeper soil layers for a few updates, before settling on a soil moisture content that was approximately 4% v/v too low in the deepest soil layer.

In these Modified Kalman-filter simulations, a standard deviation of 5% of the current soil moisture value was used. The effect of this is that when the soil moisture is high, the applied standard deviation is relatively high, and when the soil moisture is low, the applied standard deviation is relatively low. It was felt that this may be a contributing factor to the differences observed between the original and Modified Kalman-filter simulations, particularly for Soil Types 2 and 3. To investigate this, the simulation for Soil Type 2 was re-run, but with a constant standard deviation of 5% v/v. The results from this simulation are given in Figure 8.12, showing a much closer agreement between the original and Modified Kalman-filter simulations. This suggests that while some of the discrepancies seen between the Modified and original Kalman-filter simulations in Figure 8.10 and Figure 8.11 may be a result of the difference between forecasts of the correlations using the dynamics simplification approach and the original Kalman-filter, some of the discrepancy in simulation results was a result of differences in the variances applied to the forecast system states.

These analyses suggest that the Modified Kalman-filter is a good approximation to the original Kalman-filter, despite differences in the forecast correlations. Moreover, when using the Modified Kalman-filter developed in this chapter, standard deviations of the system state should be specified as a fixed value rather than a percentage of the states.

8.4 CHAPTER SUMMARY

The single most difficult operation in applying the original Kalman-filter to the spatial assimilation problem is the computation time required for forecasting of the model covariance matrix. Moreover, a full-fledged application of the extended Kalman-filter is at best a crude approximation to the actual



Figure 8.12: Soil moisture profile estimation using the Modified Kalman-filter assimilation scheme with near-surface soil moisture observations over 1 cm depth once every 5 days. Soil Type 2, standard deviations were 5% v/v.

forecast system state covariance matrix, as a result of model linearisation errors, lack of statistics concerning model error, and the initial system state covariances. In overcoming this limitation of the Kalman-filter assimilation scheme, a Modified Kalman-filter was developed, based on simplified covariance forecasting techniques. The Modified Kalman-filter forecasts the system state correlations through dynamics simplification, and assembles the forecast system state covariance matrix at update times using a specified system state variance.

Simulations using both the Modified and original Kalman-filter system state covariance forecasting have shown a good comparison between the forecasting of correlations by the two filters. Despite differences in forecast correlation of the system states, the forecasting of correlations using the dynamics simplification procedure predicted the strong correlations well and qualitatively tracked the decrease in correlation during drying periods, with a minimum amount of computational effort. Furthermore, forecasting of the system state correlations with the Modified Kalman-filter did not experience the initialisation problem displayed by the original Kalman-filter.

Simulations of soil moisture profile estimation with the Modified Kalmanfilter assimilation scheme were found to perform as well as those from the original Kalman-filter assimilation scheme, providing proper attention was paid to specification of the system state variances. It was also found that a constant system state variance performed better than a system state variance that was dependent on the system state value.

The Kalman-filter only has information about the near-surface soil layer and its correlation with deeper soil layers, and makes its adjustment of the soil moisture profile by fitting the model predictions of soil moisture content to the observed soil moisture content in the near-surface layer. Hence, when the observed and model simulated near-surface soil moisture contents are close, the Kalman-filter has no reason to believe there is any need for updating of the soil moisture profile at deeper depths.

Simulations of soil moisture profile estimation using both the original and Modified Kalman-filter assimilation schemes have shown that when the nearsurface soil layer becomes decoupled from the deep soil layer, there can be no further improvement in estimation of the soil moisture profile. This decoupling occurs during extended drying periods as a result of a divergence between the drying rates at the soil surface and deeper levels. Thus, during extreme drying events, when there is a low correlation between the near-surface and deep soil layers as a result of decoupling, the Kalman-filter is likely to perform poorly.

These simulations have highlighted the importance of "warming up" the original Kalman-filter to remove the effects of system state covariance initialisation prior to making the first update. This should then prevent the situation where a poor update is made of the soil moisture profile for the first near-surface soil moisture observation, and preventing any further improvement in the soil moisture profile estimation as a result of decoupling.