CHAPTER TWELVE

12. CONCLUSIONS AND FUTURE DIRECTION

This study has investigated the ability to estimate the spatial distribution and temporal variation of soil moisture profiles, using an approach that utilises point measurements, near-surface soil moisture observations at varying time intervals, and a hydrologic model. The hydrologic model is the kernel of the soil moisture profile estimation algorithm, as it forecasts the spatial distribution and temporal variation of soil moisture profiles during the inter-observation period. The point measurements are used for calibration of the hydrologic model and ongoing evaluation of soil moisture profile estimation. The near-surface soil moisture observations (simulating the use of remote sensing observations) are used for updating of the hydrologic model, to account for model calibration errors, spatial heterogeneities in soil parameters, precipitation and evapotranspiration.

12.1 CONCLUSIONS

The conclusions of this thesis fall into eight categories, namely: (i) the context for application of the soil moisture profile estimation algorithm and its’ influence on choosing an appropriate forecasting model and updating observations; (ii) estimation of the active microwave remote sensing observation depth; (iii) measurement of the near-surface soil moisture profile from active microwave remote sensing; (iv) synthetic study of assimilation schemes, updating frequency and updating depth; (v) development of a simplified soil moisture model; (vi) development of a simplified covariance estimation technique; (vii) one–dimensional field application of the soil moisture estimation algorithm; and (viii) three-dimensional field application of the soil moisture profile estimation algorithm. Finally, the main conclusions of the research presented in this thesis and their impact on further studies are summarised.

12.1.1 RESEARCH CONTEXT

The soil moisture data requirements govern the essential characteristics of the hydrologic model used for forecasting of the soil moisture profile distribution, and the remote sensing observations that should be used for updating of the hydrologic model. If the soil moisture data are to be used for meteorologic or climate studies, then the soil moisture profiles should be forecast with a large scale hydrologic model. This model would then be updated using either the low spatial resolution passive microwave observations, or a spatial average of the higher resolution active microwave observations. If however, the soil moisture data are to be used for more detailed hydrologic process studies or agricultural applications, then a more detailed hydrologic model with a much finer grid resolution should be used for forecasting of the soil moisture profiles. Updating of such a high spatial resolution model with active microwave observations would be more beneficial than the passive microwave observations.

As this study was interested in estimating soil moisture profiles for hydrologic applications, the scenario of updating a more detailed hydrologic model with high resolution active microwave observations was tested. Moreover, evaluation of soil moisture profile estimation, using the soil moisture profile estimation algorithm presented in this thesis, would be a more difficult undertaking for large scale model applications. This is because point measurements of the soil moisture profile have a wide variation with spatial location, and soil moisture profile estimates from large scale models provide an average soil moisture profile estimate over a large area. Even with a forecasting model resolution of 20 m, the study presented in this thesis experienced some difficulties in relating the point measurements of soil moisture content to the model estimates of soil moisture content.

This study has illustrated the improvement in estimating soil moisture profiles when near-surface soil moisture measurements are assimilated into the hydrologic model, by using data of similar characteristics to that obtained from remote sensing satellites. The soil moisture profile estimation algorithm has been developed with the direct application to remote sensing observations of near-surface soil moisture in mind. Remote sensing observations of near-surface soil moisture content were not used for assimilation into the hydrologic model, as there is still a high level of scepticism in the hydrologic community regarding the current ability to adequately measure the near-surface soil moisture content from remote sensing. Hence, this study has focussed on illustrating the usefulness of updating hydrologic models with near-surface soil moisture measurements, in terms of yielding improved estimates of the soil moisture profile.

12.1.2 REMOTE SENSING OBSERVATION DEPTH

Knowledge of the remote sensing observation depth is an essential requirement of the soil moisture profile estimation algorithm, as this is the soil profile depth for which remote sensing observations will apply. This thesis has shown that an accurate knowledge of this depth is important for the assimilation scheme to yield a good update of the hydrologic model. As there were no applicable models in the literature for estimating this observation depth for active microwave (radar) backscattering observations (for the assimilation of near-surface soil moisture content from these measurements into the hydrologic model), a radar observation depth model was developed. The theoretical amplitude attenuation observation depth model developed in this thesis estimates the radar observation depth as a function of satellite configuration (wavelength, polarisation and incidence angle) and soil moisture content.

The theoretical amplitude attenuation model presented in this thesis for estimating the radar observation depth was shown to give comparable results to experimental observations presented in literature. Furthermore, the radar observation depth was shown to be greater for *vv* polarisation than *hh* polarisation, and increases with increasing incidence angle for *vv* polarisation. Hence, the results from this observation depth model would indicate that information on the near-surface soil moisture profile may be maximised by using a low frequency sensor with *vv* polarisation and a large incidence angle. While observations depths as large as 5 cm are possible, it was shown that an observation depth of between 1 and 2 cm would be more typical of current generation remote sensing satellites.

12.1.3 REMOTE SENSING MEASUREMENT OF NEAR-SURFACE SOIL MOISTURE

Updating of the hydrologic model with near-surface soil moisture measurements from remote sensing, requires a relationship between the soil moisture content over the observation depth and the remote sensing observations. For active microwave observations, all backscattering models, apart from the Modified **I**ntegral **E**quation **M**odel (IEM), have given this relationship as a function of the average soil moisture content over this depth. As knowledge of the variation in soil moisture content over the radar observation depth for updating of the hydrologic model is more desirable than a single value, the Modified IEM would appear to be the relationship of choice. However, application of the Modified IEM was found to infer the soil moisture profile for a depth of only 3 mm, irrespective of satellite configuration and soil moisture conditions. Hence, a variation of the Modified IEM was proposed, such that it inferred the soil moisture profile for the entire radar observation depth. This involved application of a variable transition rate factor for imposing the dielectric constant profile over the observation depth.

Comparisons of backscattering simulations using the Modified IEM with a variable transition rate factor against European Microwave Signature Laboratory data showed good agreement. It was therefore concluded that a variable transition rate factor was not only feasible, but that the soil moisture profile may thus be obtained down to the observation depth, which can be as deep as 5 cm for *vv* polarisation at low frequencies.

12.1.4 ONE-DIMENSIONAL SYNTHETIC STUDY

The one-dimensional synthetic study presented in this thesis has shown that the Kalman-filter assimilation scheme was superior to the hard-update and continuous Dirichlet boundary condition assimilation schemes. For instance, it was shown that the soil moisture profile could not be retrieved for hard-updates of the surface node alone. The superiority of the Kalman-filter over the other assimilation schemes tested was through its ability to make adjustments to the deeper (unobserved) states at update times, because of the explicit correlation between soil moisture in the near-surface and deeper layers. In comparison, hard-updating can only directly alter the observed system states, relying on the internal physics of the forecasting model (eg. infiltration and exfiltration processes) to transfer information on the observed state values to the unobserved states.

The inability to directly alter more than the observed system state values with the hard-updating assimilation scheme potentially creates a mass balance problem, as the mass added during an instantaneous hard-update is restricted by the depth of the near-surface observation. In hard updating, the only source of mass to correct the mass balance errors for the entire soil profile is through the addition of sufficient mass. Two solutions to this problem were tested: (i) use a greater observation depth; or (ii) hold the observed near-surface soil moisture content fixed for some extended period of time subsequent to the actual observation (Dirichlet boundary condition).

Increased observation depths were beneficial for the hard-update assimilation scheme. However, as the near-surface soil moisture observations became less frequent, the hard-update assimilation scheme required application of the Dirichlet boundary condition.

The mass added to the system when using the Dirichlet boundary condition is constrained by the physical rate at which soil moisture can be transferred through the soil profile, and the length of time for which the Dirichlet boundary condition is maintained. Thus, the soil moisture profile estimation algorithm was insensitive to the depth of observation when the Dirichlet boundary condition was applied. Moreover, the Dirichlet boundary condition required application for an increasingly longer proportion of the update interval, in order to have the same improvement to the soil moisture profile estimation. These results have indicated that frequent observations of near-surface soil moisture content are more useful for soil moisture profile estimation than knowledge of the near-surface soil moisture content for specific periods of time.

The one-dimensional synthetic study also showed that the observation depth did not have a significant effect on the soil moisture profile estimation when using the Kalman-filter assimilation scheme. However, it was observed that unrealistic updating of the soil moisture profile can occur when near-surface soil moisture observations become less frequent, the observed and modelled soil moisture profiles are far apart, or there is a large uncertainty in the modelled profiles. This highlights the importance of frequent observations, and suggests that for the Kalman-filter assimilation scheme, repeat coverage frequency is more important than observation depth.

It was also found that the Kalman-filter always yielded stable updates of the soil moisture profile when volumetric soil moisture was modelled as the dependent state instead of matric head. The reason for this was that the volumetric soil moisture based model was a more linear form of the soil moisture profile forecasting model, meaning that it was a better approximation for forecasting of system state covariances using the extended Kalman-filter assimilation scheme. This is important, as it suggests that for application of the Kalman-filter assimilation scheme, the forecasting model must be as close to linear as possible, in order to ensure successful updating of the system forecast. Moreover, the forecasting model must have a dependence on the adjacent system states, as the Kalman-filter makes its’ update of the system based on the correlation between system states, which are evolved through the forecast model dependence on adjacent state values.

Another important conclusion from this synthetic study is that the assimilation scheme used for updating of the hydrologic model must possess the characteristics of the Kalman-filter. That is, the assimilation scheme must have the ability to directly update the entire profile, and not just the observed near-surface states.

12.1.5 SIMPLIFIED SOIL MOISTURE MODEL

The simplified soil moisture model developed in this thesis, based on a conceptualisation of the Buckingham-Darcy equation, was found to be computationally efficient and provided the necessary model for forecasting the spatial distribution of soil moisture profiles. Moreover, it was shown to be a good approximation to the Richards equation and was able to adequately simulate field measured soil moisture profiles, providing it was calibrated to an extreme drying event. This was because the model did not include a root water uptake term, which would be difficult to specify in an operation application.

12.1.6 SIMPLIFIED COVARIANCE ESTIMATION

The single most important issue in applying the Kalman-filter to the spatial assimilation problem was the computation time required for forecasting of the system state covariance matrix. In overcoming this limitation of the Kalman-filter assimilation scheme, a modification was made to the Kalman-filter forecasting of system state covariances, by applying a simplified method of estimating the covariances. A full-fledged application of the extended Kalman-filter for system state covariance forecasting is at best a crude approximation to the actual forecast system state covariance matrix, as a result of linearisation errors, lack of statistics concerning model error, and the initial system state covariances. The rationale for this was, if the essential aspects of the error dynamics can be captured by the simplified error model, the resulting loss of accuracy should be acceptable in view of the many other approximations and lack of information inherently associated with the Kalman-filter. The results of this thesis confirm this to be the case.

The modification to the Kalman-filter in this thesis involved forecasting the system state correlations through dynamics simplification, and estimation of the system state variances for assembling the forecast system state covariance matrix only at update times, not at each model forecasting time step. This is referred to as the Modified Kalman-filter.

The estimation of correlations using the dynamics simplification procedure developed in this thesis predicted the strong correlations well and qualitatively tracked the decrease in correlation during drying periods, with a minimum amount of computational effort. Despite differences in the forecast correlation of the system states with the Modified Kalman-filter and original Kalman-filter, assimilation with the Modified Kalman-filter was found to perform as well as the original Kalman-filter, providing the system state variances were correctly specified. A constant system state variance performed better than a system state variance that was linearly dependent on the state value. Another advantage of the Modified Kalman-filter is that the estimation of the system state correlations did not experience the initialisation problems observed with the original Kalman-filter.

12.1.7 ONE-DIMENSIONAL FIELD APPLICATION

A field application of the one-dimensional version of the simplified soil moisture forecasting model has shown that the assimilation of near-surface soil moisture observations with the Kalman-filter assimilation scheme was able to provide satisfactory updates of the soil moisture profile. However, it was found that the Kalman-filter updates of the soil moisture profile forecast are only as good as the forecast model's representation of the dominant soil physical processes and its calibration. When the model systematically over-predicts or under-predicts the soil moisture profile for a given near-surface soil moisture content, as the result of a model structure error, then the soil moisture profile update is likely to be poor. The reason for this is that the model indicates to the Kalman-filter that for a given near-surface soil moisture content, it should have a corresponding soil moisture profile, which is dependent on the forecasting models ability to correctly predict the soil moisture profile when the model is free from the effects of initialisation and forcing errors.

The soil porosity and residual soil moisture content are the most important soil parameters for correct estimation of the soil moisture profile. A residual soil moisture content that is too high or a soil porosity value that is too low will restrain the model from ever reaching the correct soil moisture content during extreme wet or extreme dry periods, even with an efficient assimilation scheme. Furthermore, simulation results have indicated that providing these two soil parameters have been correctly identified, the soil moisture profile may be modelled correctly during sustained dry and sustained wet periods, without assimilation of near-surface soil moisture observations. However, during dynamic wetting and drying periods, assimilation of near-surface soil moisture observations is important for correct estimation of the soil moisture profile.

It has also been shown that the Kalman-filter is unable to make any improvement in the soil moisture profile estimation when the near-surface soil layer becomes decoupled from the deeper soil layers. The reason for this is that the Kalman-filter only has information about the observed soil moisture content in the near-surface soil layer and its' correlation with deeper layers, making its' adjustment of the soil moisture profile by fitting the model predictions to the observations in the near-surface layer. Hence, when the observed and model simulated near-surface soil moisture values are close, the Kalman-filter has no reason to believe there is any need for adjustment of the soil moisture profile. Thus, during extreme drying events, when there is a low correlation between the near-surface and deep soil layers as a result of decoupling, due to divergence in drying rates, the Kalman-filter is likely to perform poorly. This is a result of near-surface soil moisture content being correctly forecast, while the soil moisture content of deeper soil layers is poorly forecast.

To ensure that the Kalman-filter does not produce a poor initial update of the soil moisture profile, particularly during periods when the near-surface and deep soil layers are decoupled, the Kalman-filter should be run for a long enough period of time to remove any effect of system state covariance initialisation. This should then ensure that the Kalman-filter makes a good initial update of the soil moisture profile as a result of an unbiased estimate of the system state covariances. The importance of this is, once the Kalman-filter makes a poor update of the soil moisture profile during periods when the near-surface and deep soil layers are decoupled, then the forecast model continues to track the correct near-surface soil moisture content. This then means that the Kalman-filter cannot make any alteration to the poor estimation of soil moisture content at deeper depths.

In addition to decoupling and model structure errors, results have shown that the Kalman-filter is also likely to perform poorly if the near-surface soil moisture observation depth is not commensurate with the depth over which the near-surface soil moisture observation is applied in the model. This is particularly important when there is a gradient in the near-surface layers of the soil moisture profile.

In conclusion, it should be noted that the Kalman-filter performed adequately for most applications of the soil moisture profile estimation algorithm developed in this thesis. Hence, the approach adopted in this thesis forms the basis of a successful data assimilation scheme for remote sensing observations of near-surface soil moisture.

12.1.8 THREE-DIMENSIONAL FIELD APPLICATION

Application of the Modified Kalman-filter assimilation scheme to the Nerrigundah catchment, using the three-dimensional version of the simplified soil moisture profile forecasting model, has shown that the soil moisture profile dynamics of a small experimental catchment could be adequately estimated using the soil moisture profile estimation algorithm developed in this thesis. By using such an algorithm, the influences of poor initialisation of the soil moisture model were overcome, yielding an average rms error in total soil moisture storage of 6% v/v, as compared to 13% v/v when near-surface soil moisture observations were not assimilated into the soil moisture model.

In the rare situation where there is a good initialisation of the soil moisture forecasting model, the forecasting model has a good calibration, and high quality forcing data is available, updating of the model with near-surface soil moisture observations was found to slightly degrade the otherwise excellent estimation of the soil moisture profile dynamics. This was a result of noise in the near-surface soil moisture observations, and the application of observation noise and system state variances in the Modified Kalman-filter. However, when the initialisation of the soil moisture profile forecasting model was poor, as is the usual situation, assimilation of near-surface soil moisture observations into the forecasting model made an obvious improvement in the soil moisture profile estimation.

Simulation results have also indicated that when near-surface soil moisture observations are of low quality, and this is not reflected by the observation variances, estimation of the soil moisture profile may be poor. This suggests that the assimilation of near-surface soil moisture observations into a hydrologic model should yield an overall general improvement in the estimation of spatial distribution and temporal variation of soil moisture profiles, providing the near-surface observations are of sufficient accuracy.

With an improved application of the forecast system state variances and observation variances, the estimation of soil moisture profiles may be further improved, particularly when the simulated and observed near-surface soil moisture content values are already close. This study has also highlighted the difficulty of relating point measurements of soil moisture content to the spatially averaged estimates from a soil moisture model. Hence, evaluation of the soil moisture profile estimation algorithm is likely to be the most difficult component of soil moisture profile estimation over large areas.

Simulation results have also shown that adequate estimation of the soil moisture profile was not heavily dependent on the frequency of near-surface soil moisture content measurements. However, this is provided the model calibration and forcing data are of sufficient accuracy, with poor estimation of the soil moisture profiles being only a result of poor initialisation of the forecasting model. When calibration errors exist in the forecasting model, or more importantly, there are significant errors in the forcing data, then the effect of the update interval will be influenced by the rate at which the forecasting model dynamics result in a divergence from the correct simulation of soil moisture profiles.

12.1.9 SUMMARY OF MAIN CONCLUSIONS

This thesis has developed a methodology for estimating the observation depth of near-surface soil moisture measurements from active microwave remote sensing. Moreover, a procedure has been developed for inferring the near-surface soil moisture profile over the observation depth, from active microwave observations. This provides the essential input for updating of the soil moisture model in an operational setting.

A soil moisture profile estimation algorithm has been developed for estimating the soil moisture dynamics of a small catchment. This has involved the development of a computationally efficient soil moisture profile forecasting model, and a computationally efficient application of the Kalman-filter assimilation scheme, by developing a simplified procedure for forecasting the system state covariances. Moreover, it has been shown that an assimilation scheme which has the characteristics of the Kalman-filter is required for effective updating of the soil moisture forecasts, and that the forecasting model must be as near to a linear representation of the soil physics as possible, to ensure stable updating of the model. However, updating of the soil moisture profile is only as good as the forecasting model’s representation of the soil physics. Furthermore, it is necessary to have an accurate knowledge of the depth for which near-surface soil moisture measurements relate, when updating the soil moisture model.

12.2 FUTURE DIRECTION

Recommendations for future research fall into five categories, namely: (i) estimation of the remote sensing observation depth; (ii) measurement of the near-surface soil moisture profile from remote sensing; (iii) forecasting of soil moisture profiles; (iv) system state variance specification in the Modified Kalman-filter; and (v) advances towards operational estimation of the spatial distribution and temporal variation of soil moisture profiles. Potential research in each of these five categories is addressed below.

12.2.1 REMOTE SENSING OBSERVATION DEPTH

Whilst the radar observation depth model developed in this thesis agreed well with experimental observation depth values noted in literature, it has not been widely evaluated. Hence, it is proposed that a ground based experimental program could be designed to evaluate the theoretical remote sensing observation depth model from backscattering observations. Such an experiment would involve making backscattering observations of a soil surface for different soil moisture contents, wave polarisations and incidence angles, with a metal plate inserted at incrementally increasing depths. The metal plate would provide a dielectric discontinuity in the soil, which would have a strong backscattering response when located within the radar observation depth. Once the plate insertion depth is increased beyond the radar observation depth, there would be a significant reduction in the total backscattering observed by the remote sensor.

12.2.2 REMOTE SENSING MEASUREMENT OF NEAR-SURFACE SOIL MOISTURE

Although the proposed variation on the Modified IEM allows the near-surface soil moisture profile over the observation depth to be measured, it still contains restrictive assumptions regarding the dielectric constant imposed for evaluation of the modified reflection coefficients. By replacing the modified reflection coefficients with an approximate solution to the Riccati equation, the

Modified IEM may be applied to any dielectric profile shape. This would eliminate the imposed transition of the dielectric profile in the near-surface air layer when using the modified reflection coefficient. It is proposed that application of the reflection coefficients from the Riccati equation in the Modified IEM be evaluated with backscattering data collected at the European Microwave Signature Laboratory.

In addition to the above, application of the Modified IEM for measuring near-surface soil moisture content in the field may be evaluated from the two ERS-2 remote sensing data sets obtained during the intensive field campaign in this thesis, and comparison made with the ground measurements. Moreover, the significance of local incidence angle on inferring the near-surface soil moisture content from backscattering observations with the Modified IEM, may be evaluated by using the two DEM data sources presented and by assuming a flat surface.

12.2.3 SIMPLIFIED SOIL MOISTURE MODEL

It has been shown that unless the simplified soil moisture profile forecasting model was calibrated to extended drying periods, soil moisture in the deep soil layers was forecast incorrectly, as a result of the neglect of a root water uptake term. However, in simulating field measured soil moisture profiles by calibrating to extreme drying events without the root water uptake term, soil parameters no longer had the physical meaning intended. Hence, a root water uptake term should be added to the model, to account for transpiration during periods when evapotranspiration rates exceed the rate of capillary rise to the upper soil layer.

12.2.4 SIMPLIFIED COVARIANCE ESTIMATION

Soil moisture profile estimation using the Modified Kalman-filter was shown to produce poor updates of the near-surface soil moisture in some instances, particularly when model forecasts and observations were already close. This was a result of strong lateral correlations with adjacent observations that had a large difference in soil moisture content between the model forecast and the observation, and the specification of a constant system state variance. Hence, it is suggested that rather than using a constant system state variance, the Modified Kalman-filter update might be improved by estimating the system state variance from the difference between the observed and forecast estimate of near-surface soil moisture content, and the variance of the observation.

12.2.5 OPERATIONAL SOIL MOISTURE PROFILE ESTIMATION

The emphasis of this thesis has been on identifying an appropriate methodology for estimating the spatial distribution and temporal variation of soil moisture profiles, through the assimilation of near-surface soil moisture observations from remote sensing in an operational setting. Hence, the obvious progression from the work established in this thesis, is to test the soil moisture profile estimation algorithm with actual remote sensing data. Moreover, the effects on soil moisture profile estimation from errors in published elevation data, published soils data, and forcing data from only routinely collected meteorological observations should be investigated.

In addition to the above, it has been shown in this thesis that microwave remote sensing of near-surface soil moisture content is heavily dependent on the soil temperature, through the relationship of volumetric soil moisture content with dielectric constant. Hence for remote sensing observations to be useful for measuring the near-surface soil moisture content, the spatial distribution and temporal variation of soil temperature profiles must be estimated, in addition to soil moisture. This has not been thoroughly investigated here, other than for the one-dimensional synthetic study.

Apart from providing absolute values of near-surface soil moisture content, remote sensing data can be used to estimate the change in near-surface soil moisture content between successive observations through the method of change detection. The inclusion of this type of data for updating of the hydrologic model has not been evaluated. Furthermore, point measurements of soil moisture content may be used to update the hydrologic model at discrete points. However, through lateral correlations in the forecasting model, updating of the model may be made for more than just the observed point. Likewise, near surface soil moisture observations for only part of the model domain may provide updating information for more than just the observed portion of the catchment, as a result of lateral correlations in the model. Moreover, point measurements of soil moisture may be used to interpolate the spatial measurements of near-surface soil moisture content, to provide updating information over the entire soil profile, with an obvious increase in its uncertainty. This type of information may alleviate the effect of decoupling on the Kalman-filters ability to make corrections to the soil moisture profile estimation.