6. VALIDATION AND VERIFICATION

Development of the hydrosalinity module of *ACRU, viz. ACRUSalinity* is followed by validation and verification of output from the module to see how it performs under field conditions. The validation process involved code validation followed by verification of simulated results through comparison against observed data from the Upper Mkomazi Catchment in KwaZulu-Natal province, South Africa.

Scientists and decision makers need assurances that the model they apply is valid. According to McLaughlin (1988), from a technical or scientific point of view a model is validated when it properly describes the physical processes. From a regulatory point of view, however, it is validated when the model yields adequate predictions with the main goal being to reduce the risk of making inappropriate decisions from the model results. Loague *et al.* (1998) suggest that a model is a good representation of reality, and hence valid, if it can be used to predict certain observable phenomena within acceptable accuracy and precision. However, according to Herald (1999), there is no defined procedure or technique that is widely accepted to do this. Furthermore, the level of acceptable inaccuracy will vary with applications. Hence, one model may be valid for a situation requiring general trends and qualitative information, such as irrigation management and educational purposes, but invalid for pure scientific research.

The approach employed to validate the hydrosalinity module of *ACRU* involved salt balance computations for different components with the help of a spreadsheet. This was done to validate the algorithms underlying the various hydrosalinity processes in terms of mass conservation. This step is not intended for generating outputs to be used for comparison against the observed data. Therefore, some of the salinity related inputs to the model were hypothetical values. The approach to verify the model's output involved use of hydrological and salinity related data specific to the Upper Mkomazi Catchment and the model outputs are graphically and analysed statistically for comparison against observed data. This chapter therefore presents the following:

- A general description of the Upper Mkomazi Catchment
- Code validation of the *ACRUSalinity* module and

- Verification through comparison of model output against observed streamflow salinity data.

6.1 Description of the Upper Mkomazi Catchment

The Upper Mkomazi Catchment constitutes the upstream part of the Mkomazi Catchment draining to the U1H005 weir (flow gauge). The Mkomazi Catchment is located in KwaZulu-Natal province in South Africa. The Upper Mkomazi Catchment is used during the evaluation phase of the hydrosalinity module of *ACRU* which is developed in this project. Although, salinity is not a threat to this catchment, some of the criteria considered when selecting the catchment are:

- The entire catchment was previously configured for *ACRU 300* version of the *ACRU* model (Taylor, 2001) and
- In comparison with many of the other catchments that are configured for the *ACRU* model (including the Lower Mkomazi Catchment), this catchment has good streamflow TDS concentration data.

What follows is a general description of the Upper Mkomazi Catchment. Detailed information about the catchment can be obtained from reports of other studies undertaken for the area, e.g. Dickens (1998), IWR (1998) and Taylor (2001).

6.1.1 Climatological and hydrological conditions

Climatically the Mkomazi Catchment is classified as a humid zone (IWR, 1998). Rainfall distribution is reasonably consistent throughout the catchment, ranging from nearly 1300 mm per annum (p.a) at the headwaters to 1000 mm p.a in the middle and 900 mm p.a in the lower reaches of the catchment. The Mean Annual Precipitation (MAP) for the entire catchment is 981mm. However, the MAP is higher in the upstream parts of the catchment (1000-1287 mm) and correspondingly most of the runoff is generated upstream (IWR, 1998). The mean monthly A-pan equivalent evaporation ranges from a minimum value of 59 mm for June to a maximum of 150 mm for December (Schulze, 1997).

The Mkomazi River flows from the foothills of the Drakensberg Mountains towards the east. Two streamflow gauges with flow records dating from early 1960s exist along the river. The first, U1H005 commands the upstream part of the catchment (1744 km^2) and the second, U1H006 is close to the estuary (4349 km^2) and records flow from the entire catchment. The historical records for the upstream gauge (Figures 6.1, 6.2) have few gaps due to missing data. The downstream gauge, however, has unreliable high flow measurements (IWR, 1998).

Figure 6.1 The U1H005 gauging weir at Camden

Figure 6.2 Mkomazi River from upstream of the U1H005 gauging weir

6.1.2 Physiography

The great Escarpment around Sani Pass forms the headwaters of the Mkomazi, which exits into the Indian Ocean at Umkomaas (IWR, 1998). Table 6.1 provides some sub-catchment physiographic information of the Upper Mkomazi Catchment. The catchment's altitude ranges from 2165 m in the north western part of the catchment (sub-catchment 5) to 1339 m in the south eastern part of the catchment (sub-catchment 14).

Table 6.1 Sub-catchment physiographic information of the Upper Mkomazi Catchment (after Taylor, 2001)

Sub-catchment No	Longitude (degree, decimal)	Latitude (degree, decimal)	Area (km^2)	Mean Altitude (m)
1	29.38	29.51	162.91	2124
2	29.39	29.59	63.32	1959
3	29.54	29.58	141.69	1533
4	29.64	29.61	29.22	1373
5	29.49	29.41	142.97	2165
6	29.46	29.47	57.76	2088
7	29.60	29.50	208.01	1639
8	29.71	29.59	47.09	1410
9	29.71	29.49	189.23	1851
10	29.79	29.56	77.44	1643
11	29.38	29.62	93.12	2104
12	29.60	29.71	32.87	1685
13	29.60	29.69	148.15	1568
14	29.79	29.64	29.97	1339
15	29.90	29.60	18.87	1680
16	29.84	29.64	70.94	1492
17	29.71	29.72	69.99	1678
18	29.81	29.72	158.55	1310

6.1.3 Land use and land cover

Under natural conditions, the upper catchment vegetation would be dominated by pure grassveld and temperate and transitional forest and scrub, with false grassveld and coastal tropical forest dominating the middle and lower catchment (IWR, 1998). However, a survey conducted by Edward (1998) has shown that the Mkomazi Catchment is a highly modified one due to excessive levels of utilisation. As a consequence of this disturbance, the river system has been heavily infested with alien plant species and the diversity of the riparian vegetation has been drastically reduced. The riparian zone is characterised by considerable infestation of wattle which has resulted in a loss of the local riparian species. This phenomenon was noticed during the field visits undertaken by Taylor in 2001 and by the author in 2003. Only a few remnants of the riparian vegetation remain. The large number and diversity of pioneer species indicates high levels of disturbance (Edward, 1998).

The present land use from satellite imagery in 1996, which was used previously as input to the *ACRU* model for hydrological simulation of the Mkomazi Catchement, includes a number of land use categories (Taylor, 2001). Land use classes of the Upper Mkomazi Catchment are shown in Figure 6.3. As it can be seen from the figure, the Upper Mkomazi Catchment is mainly dominated by unimproved grassland but with a significant proportion of the area being degraded due to overgrazing coupled with the steep gradient of the landscape. Forest plantations and subsistence dryland agriculture are other land uses in the catchment. Human activity along the river varies from low in the upper reaches, to diverse agriculture in the middle to lower reaches.

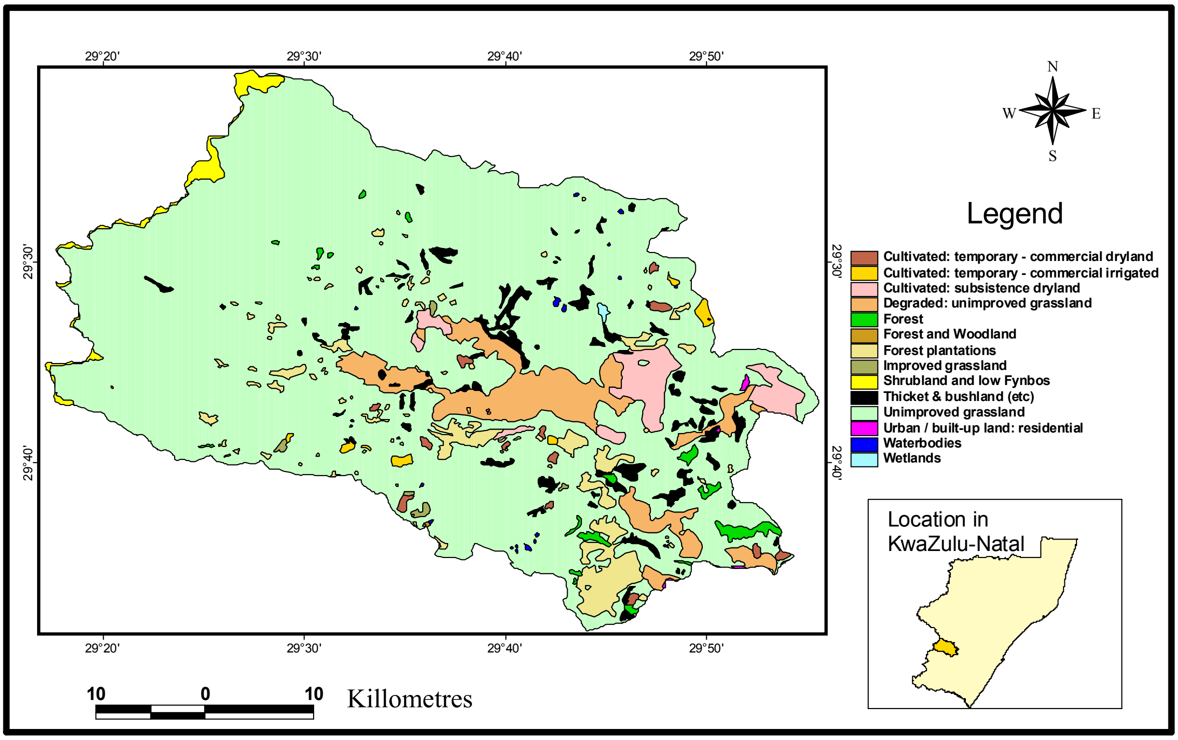


Figure 6.3 Land use classes of the Upper Mkomazi Catchment (after Taylor, 2001)

6.1.4 Geological formations

The Upper Mkomazi contains a wide range of geological formations from igneous rocks in its upper reaches to sedimentary rocks in its middle and lower reaches. The upper part of the catchment is dominated with Basalts and Arenites. Mudstones occupy most of the middle and lower part of the catchment's geology. Dolerite also characterises the middle lower part of the catchment's geology. According to Rowntree and Dollar (1998), the faulted terrain feature of the catchment signifies structural control of the channel and the effect of basement geology can be noticed from the general relief. The upper catchment has steep relief, while the middle and lower-middle catchment can be classified as undulating. Steep relief in the lower part of the catchment is a function of the undulating lithology. The lithology produces clay to clay loam soils (Rowntree and Dollar, 1998). Figure 6.4 shows major geological formations in the Upper Mkomazi Catchment.

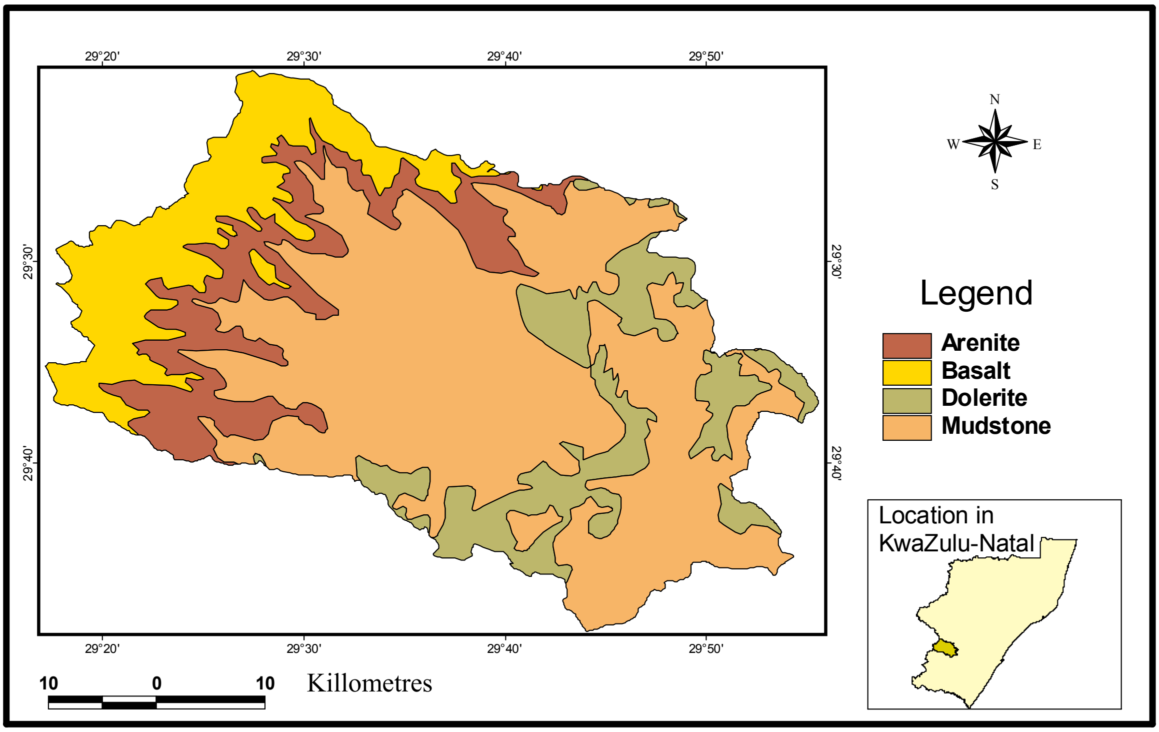


Figure 6.4 Major geological formations of the Upper Mkomazi Catchment (after Council for Geoscience, 1999)

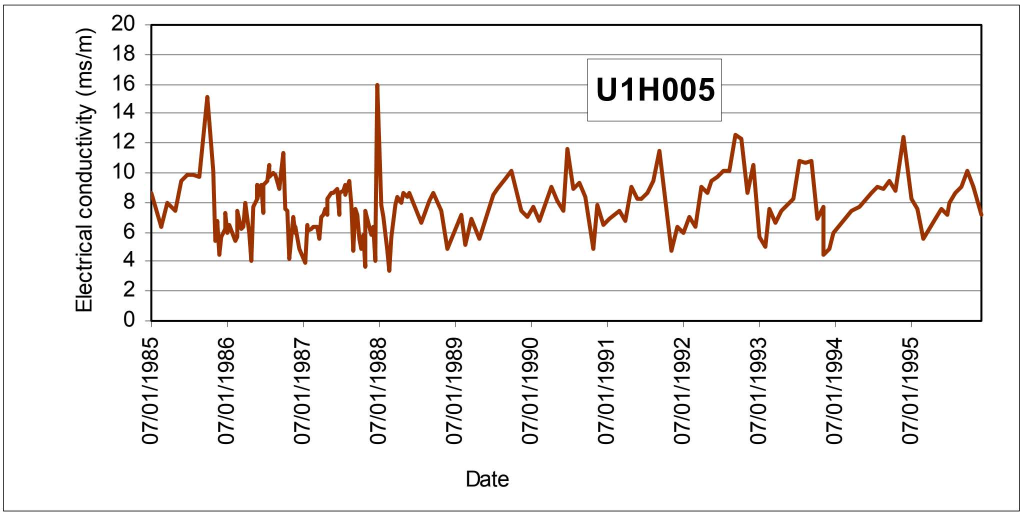
6.1.5 Salinity in the catchment

The current levels of salinity in the Upper Mkomazi Catchment are not a threat for most uses of the water in the catchment. However, the increased TDS concentration of water flowing at the catchment outlet compared to rainfall TDS concentration in the catchment implies that both natural and anthropogenic factors are causing an impact that generally results in the differences in TDS concentration between the rainfall and outflowing water.

The natural and human-induced salinity in the catchment result from point and non-point sources. The natural sources of salinity in the catchment generally originate from the weathering and dissolution of underlying rocks or soils overlying the rocks. Although, when compared to the lower parts of the Mkomazi Catchment, the Upper Mkomazi Catchment is influenced less by human activities, agricultural land use still constitutes a substantial part of the catchment. Agricultural practices in the catchment may result in increased salt concentrations and salt loading in draining streams. Total evaporation from crops result in concentrating dissolved solids in the remaining return flows. Irrigation practices also increase the flow through soils, which is expected to increase the total salt loading from previous natural salt loading levels.

DWAF salinity data from 1985 to 1995 that included EC values for weirs U1H005 and U1H006 have been assessed to identify seasonal fluctuations and any general long term trend. The results are shown in Figure 6.5. The EC values do not show significant increases with time at either weir. Seasonal fluctuations in EC, however, are evident at both stations, mainly as a result of seasonal changes in natural processes. During the rainy season, TDS concentrations drop due to the dilution effect of rain falling on the area, whereas during the dry season salt concentration starts to increase due to the “evapoconcentration” processes. The comparison of EC values between U1H005 and U1H006 weirs has shown that TDS concentrations increase downstream in the catchment. This can be attributed to the re-use of water as it flows downstream and due to the increased human influences in the lower parts of the catchment.

In general, this assessment of historical EC data between the period of 1985 to 1995 for both the upper and lower sampling sites (U1H005 and U1H006 respectively) did not show any significant increases with time. However, the seasonal fluctuations in EC values observed in both stations are in response to changes with time of natural and/or anthropogenic factors influencing the hydrosalinity processes. Hence, any activity that facilitates these processes would possibly increase the currently low streamflow TDS concentrations of the catchment to an extent that could limit the domestic and/or agricultural and/or industrial uses of the water.



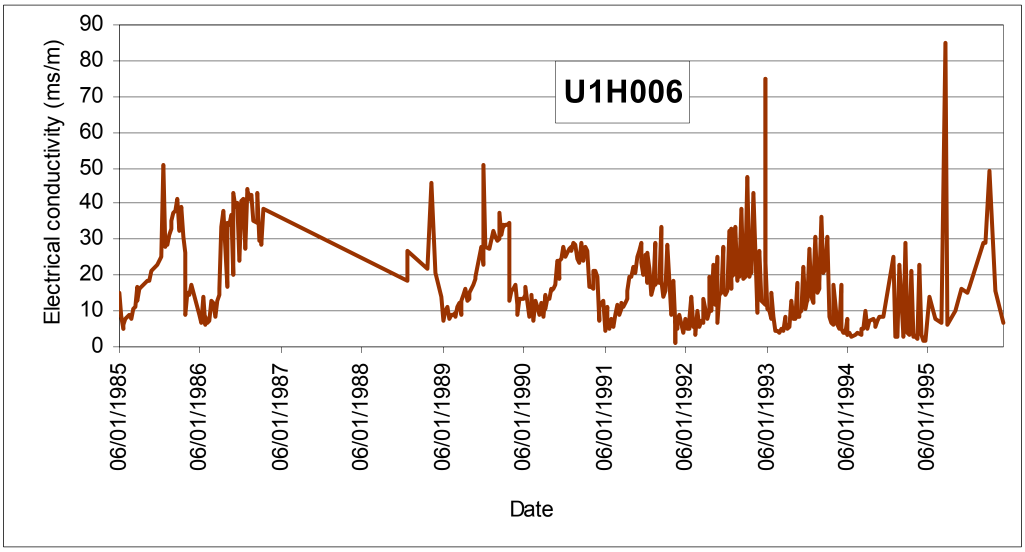


Figure 6.5 Intra-and inter-annual trends of streamflow salinity in the Upper (U1H005) and Lower (U1H006) Mkomazi Catchments

6.2 Previous Modelling Efforts in the Upper Mkomazi Catchment

Some researchers have conducted modelling based hydrological studies in the Mkomazi Catchment. These studies, undertaken by DWAF and the School of Bioresources Engineering and Environmental Hydrology at the University of Natal include detailed modelling studies in the catchment and are outlined below.

6.2.1 DWAF pre-feasibility study

A general pre-feasibility study was conducted in the Mkomazi Catchment by DWAF for the Mkomazi-Mgeni Transfer Scheme. The objective of this study was to select an optimal transfer scheme for the Mkomazi through identification and evaluation of a number of potential schemes, eliminating those that have little merit, and carrying out a reconnaissance survey of the remaining schemes (NSI, 1998).

The study includes modelling present and future scenarios on the impact of domestic, agriculture, forestry, industrial as well as environmental demands on the available water resources. The hydrological models employed in the study were the Water Resources Yield Model (WRYM) and the BKS AFFDEM program for modelling forestry demands. This study disaggregates the Mkomazi Catchment into the 12 DWAF Quaternary Catchments in order to model the impact of forestry and irrigation at this level of spatial disaggregation. Furthermore, this study of DWAF investigated various water resources development schemes such as the Impendle and Smithfield dam schemes and their potential hydrological impact on downstream water resources.

6.2.2 *ACRU* based simulation study

A comprehensive hydrological modelling study using the *ACRU* model was conducted by Taylor (2001) with the general aim of assessing water resources management scenarios in the Mkomazi Catchment. The simulation includes daily flows for use in assessing the streamflow characteristics associated with the in-streamflow requirements. The study also includes modelling the impacts of land use change and water resources development on the availability of water resources. This study delineates the Mkomazi Catchment into 52 sub-catchments. This was done in order to represent the different land use and management practices as discrete units as well as considering proposed developmental concerns within the catchment (Taylor, 2001).

6.3 Setup of *ACRU2000* For the Upper Mkomazi Catchment

As stated in Section 6.2.2, the *ACRU* model was previously configured for the Mkomazi Catchment by Taylor (2001). This configuration of the *ACRU* model for the Mkomazi Catchment, through further refinements of the 12 Quaternary Catchments, delineates the whole Mkomazi Catchment into 52 sub-catchments. The first 18 sub-catchments representing the Upper Mkomazi Catchment are shown in Figure 6.6. Figure 6.7 also shows the flow direction and thus salt transport route between sub-catchment cells.

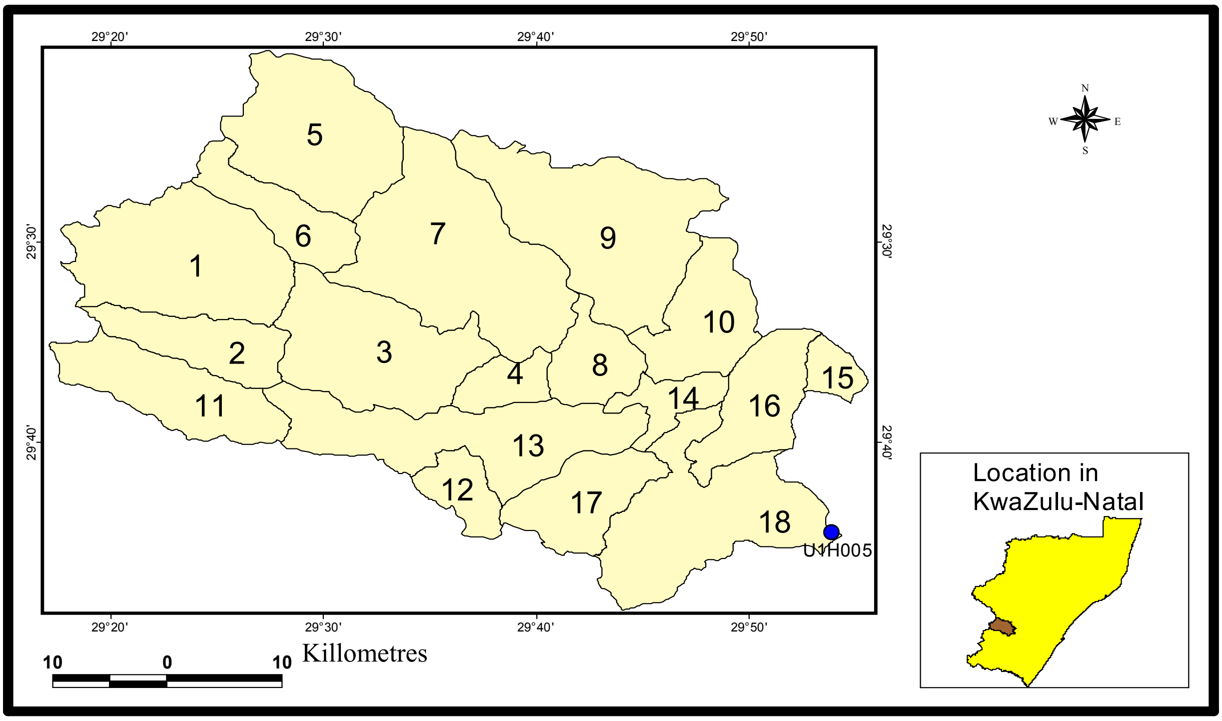


Figure 6.6 *ACRU* sub-catchment delineation of the Upper Mkomazi Catchment (after Taylor, 2001)

The Mkomazi Catchment was configured for the FORTRAN based *ACRU 300 series*. The *ACRU 300 series* uses a single Menu file that holds most of the input data information for all sub-catchments and hydrological response units. *ACRU2000,* there against, requires a separate input file for each hydrological response unit within a sub-catchment and a control file that holds general information about the simulation such as sub-catchment specifications and the start and end dates of simulation. Thus the *ACRU* Menu file was converted to *ACRU2000* input files and a control file using one of the *ACRU* Utilities, *viz.* the *ACRU* Menu Converter program.

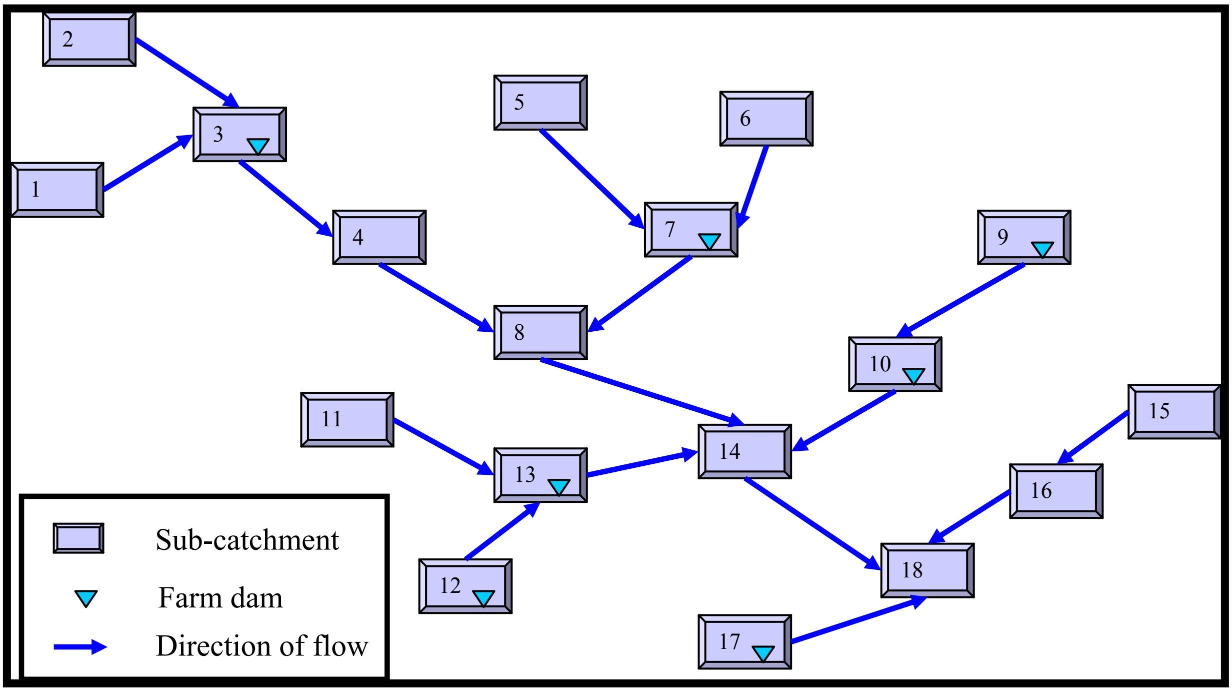


Figure 6.7 Diagram of sub-catchment configuration for the Upper Mkomazi Catchment (after Taylor, 2001)

Each sub-catchment of the Mkomazi Catchment is composed of nine hydrological response units (land use categories) as shown in Table 6.2. In *ACRU2000* each of these units has its own input file. Therefore, for the first 18 sub-catchments included in the Upper Mkomazi Catchment, a total of 162 input files (18 x 9) are generated from the original Menu file. The input parameters specific to *ACRUSalinity* are then added at the end of each of the 162 input files in accordance with the *ACRU2000* input format.

Table 6.2 Hydrological response units in each sub-catchment of the Upper Mkomazi Catchment (after Taylor, 2001)

Sub-catchment No	Total area (km^2)	Forest (km^2)	Plantation (km^2)	Valley Bushveld (km^2)	Dryland (km^2)	Urban (km^2)	Grassland (km^2)	Wetland (km^2)	Channel (km^2)	Dams & Irrigation (km^2)
1	162.914	0.000	0.401	0.866	0.000	0.000	160.538	0.000	1.095	0.010
2	63.323	0.000	0.806	0.000	0.000	0.000	61.635	0.000	0.867	0.010
3	141.668	0.000	6.659	4.196	0.636	15.269	113.357	0.000	1.535	0.032
4	29.216	0.000	1.952	0.833	0.000	17.551	8.156	0.000	0.712	0.010
5	142.968	0.237	0.000	0.000	0.000	0.000	141.636	0.000	1.081	0.010
6	57.758	0.825	0.173	0.000	0.000	0.000	55.799	0.000	0.946	0.010
7	208.006	0.268	2.804	12.608	5.258	11.196	172.560	0.946	2.712	0.597
8	47.091	0.000	0.000	0.046	0.007	25.206	20.334	0.000	1.484	0.010
9	189.227	0.000	0.545	5.806	0.649	0.000	179.017	0.000	1.464	0.801
10	77.443	0.000	4.191	1.879	19.236	4.029	44.327	0.000	1.137	2.641
11	93.123	0.208	1.569	0.000	0.000	0.000	89.965	0.000	1.367	0.010
12	32.865	0.140	0.606	0.000	1.084	0.000	29.126	0.000	0.360	1.546
13	148.147	0.000	12.190	1.323	4.685	0.318	123.587	0.000	2.144	3.898
14	29.970	0.000	2.026	0.289	6.071	3.478	17.607	0.000	0.487	0.010
15	18.867	0.000	0.001	0.000	10.052	0.229	8.378	0.000	0.195	0.010
16	70.939	1.337	0.422	7.124	1.990	8.517	50.614	0.000	0.924	0.010
17	69.655	1.214	3.213	3.537	0.350	0.351	59.695	0.000	0.618	0.676
18	158.546	8.802	27.145	7.589	2.276	22.561	86.517	0.000	3.644	0.010

6.4 Basic Data Input Requirements and Data Preparation for *ACRUSalinity*

Model predictions are commonly compared with measured data in order to prove that the model output is a realistic representation of field processes. However, in order to compare model simulations with measured data, model input parameters must be known and field data to compare with model outputs must also be available. Thus, the first step towards the verification phase was to obtain the required raw data inputs and subsequent preparation of these data in a way that can be used by the model. Data relating to the hydrological aspect were already available. However, data that are specific to the new module (*ACRUSalinity*) still needed to be input. These were obtained from various sources. The following sections will discuss the methodology followed and the assumptions taken to derive values of particular parameters.

6.4.1 Rainfall and irrigation water TDS concentrations

As described in Section 2.2.2, rainfall is the fundamental driving force and pulsar input to most hydrological processes (Schulze *et al.*, 1995c), resulting also in water quality impacts from non-point sources (Pegram and Görgens, 2001). Rainfall plays a major role during wet atmospheric deposition. This is particularly true in areas with low salinity waters. In such areas the chemical composition is controlled mainly by the amount of dissolved salts furnished by precipitation. On the other hand, rainfall has a dilution effect on areas with high TDS concentration.

Salt input to the topsoil of irrigated and non-irrigated lands is computed in *ACRUSalinity* from the volume of rainfall and irrigation water as well as their associated TDS concentrations. This module assumes a single average representative rainfall salt concentration value for each sub-catchment. Analysis of rainfall samples by Simpson (1991) collected over a period of seven months at Cedara meteorological station (located in U2H016 catchment) in the neighboring Mgeni Catchment reveals that the average TDS concentration on the area to be 11.3 mg/l. The measured rainfall TDS concentration ranges from 2.7 mg/l to 27 mg/l. A similar study carried out by Flügel (1995) in the Western Cape province from an analysis of 67 rainfall samples has shown rainfall salt concentrations varying between 14 and 125 mg/l with an average value of 37 mg/l. Görgens (2003) suggests that rainfall TDS concentration of the Mkomazi Catchment would be lower than the Western Cape province.

Therefore, based on the above information the rainfall TDS concentration of the Mkomazi Catchment is assumed to have the same value as its neighboring Mgeni Catchment, and as measured at the Cedara meteorological station. Hence, a value of 11.3 mg/l is taken as the average rainfall TDS concentration for the Upper Mkomazi Catchment. Similarly, no data was found for the catchment's irrigation water TDS concentration. Hence, assuming the main source of irrigation water supply in the catchment to be from the river, the average TDS concentration of streamflow at U1H005 *viz.* 58 mg/l, is taken as a representative value.

6.4.2 Initial TDS concentrations of subsurface and reservoir water storage

In *ACRU*, the initial soil water content of the topsoil and subsoil at the start of a simulation are input to the model. Therefore, in order to account for the impact of this subsurface water storage at the start of a simulation on surface and subsurface TDS balance, it is important to determine the salt load associated with the initial soil moisture. The initial salt load of these subsurface systems is computed and set before any of the other hydrosalinity processes are executed for the simulation period. From assessment of the historical record of the streamflow salinity, the average maximum value during the dry season was found to be 100 mg/l. Therefore, based on the assumption that streamflow during the dry season is composed of only subsurface flow and hence its salinity reflects the average TDS concentration of the subsurface system, the initial salt concentration of the topsoil and subsoil is taken as 100 mg/l. A sensitivity test of this variable has shown that the impact of this variable on surface and subsurface TDS balance decreases with time and it would have little effect after three months (Section 7.1.3). Therefore, a warm up period of three months is also used in all simulations to minimise errors emanating from data uncertainty of the initial TDS concentration.

ACRU also considers the initial volume of water stored in reservoirs at the start of a simulation. Thus, in order to conserve the salt mass, *ACRUSalinity* also computes and stores the initial salt load of a reservoir at the start of a simulation. This salt load is computed from the initial volume of water stored in the dam and its salinity which is input to the model by the user. Hence, the initial TDS concentration of a reservoir needs to be known. For the purpose of this dissertation this value is assumed to have the same value as the streamflow average TDS concentration. Therefore, the initial stored water in the reservoir at the start of simulation is assumed to have TDS concentration of 58 mg/l. Similar to that of initial subsurface TDS concentration, the initial reservoir water TDS concentration value was also found to have little effect on simulated daily TDS concentration values after a few days following the start of the simulation (Section 7.1.4). This is particularly true for small reservoirs draining big catchment areas where the whole initial storage of the reservoir may even get replaced with "new" water after only few high events.

6.4.3 Salt uptake rate and equilibrium values

ACRUSalinity uses a first order rate kinetics equation to describe the salt generation process in subsurface components. Data requirements of this process include the salt concentration of the specific layer before salt generation, the equilibrium value (saturation value) and the rate constant. The first parameter is calculated internally from the daily salt and water balances. The equilibrium value and the rate constant, however, are inputs to the model.

Estimated values of these parameters can be determined if daily soil salinity data are available for the area. However, no such time series records are found for the Mkomazi Catchment. An attempt was made to derive estimated values for the salt uptake rate constant parameter from the available streamflow salinity records measured during the dry season. This is based on two basic assumptions. First, during the dry season the streamflow is composed of only subsurface flow and hence, during this period, the streamflow has the same salt concentration as the subsurface water. Secondly, the Upper Mkomazi Catchment is less influenced by human activity, thus there is little or no effluent discharge to the stream. Historical streamflow and salinity data in U1H005 are then assessed to extract data that can fulfill the abovementioned requirements.

Regression analysis based on the extracted data sets was conducted with the help of GENSTAT Software (McConway *et al.*, 1999). The data sets are fitted into the first order rate kinetics equation in the form of Equation 3.9 and assuming a C_e value of 3000 mg/l (a lower range of the global average maximum soil salinity values (Aswathanarayana, 2001)). The difference between this maximum soil salinity and the daily salinity values is then treated as the explanatory variable (x). Similarly, the difference in TDS concentration between successive days is treated as the response variable (y). Further, the y-intercept term is omitted from the model to express the equation in its original form. The GENSTAT output for this analysis is shown in Appendix F. Output from this regression analysis shows that, the slope of the curve that represents the rate constant, k, is $3.4 * 10^{-4}$ at a significance probability of less than 0.001 and standard error of observations of 0.534. Both parameters indicate that the first order rate kinetics model is adequate to describe the increase in streamflow TDS concentration with time. The regressed *k* value is also not far from the range of theoretically expected values of this parameter (i.e. 10^{-4} - 10^{-7} day^{-1}) for individual solute species, as suggested by Ferguson *et al.* (1994). However, the regression analysis has shown an extremely low accounted percentage of variance. This can be attributed to the low number of observations used in the regression analysis (only 15 records), due to limitations in the availability of daily streamflow TDS concentration data recorded between two rainfall events. Therefore, it was decided that the rate constant and equilibrium values had to be derived by calibration against observed TDS values.

6.5 Code Validation of the Major *ACRUSalinity* Process Objects

One measure of model validity is the ability of the model to conserve mass (Konikow, 2002). This can be measured by comparing the net fluxes calculated or specified in the model, e.g. inflow and sources minus outflow and sinks with changes in storage (accumulation or depletion). The mass balance computations can thus be used to assess whether the algorithms describing various processes yield the desired results.

It is time intensive to make a detailed code validation of the algorithms underlying each process in the module. Therefore, this section validates the code underlying only the key processes which might likely have errors due to the relatively complicated algorithms describing them. This mainly occurs on these processes that involve transport of salts from one component to another, or that receive TDS concentration or salt load information from two or more components. However, during the development process of the hydrosalinity module, mass balance computations were done after every change or new addition made to process objects, so as to track and correct such errors over time.

6.5.1 Code validation of subsurface salt movement processes

Mass conservation computations in any of the subsurface components consider salt gains (inflows) to, and losses (outflows) from, the components under consideration. *ACRUSalinity* assumes that the sources of salt gains to a subsurface component (a soil horizon or the groundwater store) are:

- salt input through wet atmospheric deposition (rainfall salt input)
- salt input from applied irrigation water, and
- salt generated as a result of *in situ* weathering processes.

The term salt input in the Table 6.3 and 6.4 refers to the salt input from both irrigation and rain water. Similarly, losses from any of the subsurface components are assumed to be as a result of:

- downward salt transport associated with the saturated downward flow of water
- salt load associated with baseflow release, in the case of groundwater system, and
- upward salt transport along with upward saturated flow of water.

The mass of salt stored on a particular day in any of the subsurface components (topsoil, subsoil or groundwater store) is computed from consideration of the previous day's salt load, gains to the system and losses from the system as follows:

calculated current salt load = previous day's salt load + total gain - total loss

Outputs obtained from the model are used for these mass balance computations, as shown in Tables 6.3 and 6.4. The salt load associated with the upward flow of water for the three consecutive days selected for this computation was zero. The salt input column, for the case of topsoil refers to the salt load added from rainfall or irrigation water, whereas, for subsequent layers, it refers to salt load associated with percolation water from the overlying layer.

The calculated current salt load is compared against the simulated value and the error is then expressed as a percentage difference between the calculated and simulated values. Only minor differences (of an order of less than 10^{-9}) between calculated and simulated values can be noticed from the "Error" column of both tables. This is attributed to rounding errors.

Table 6.3 Mass balance for code validation of subsurface salt movement processes in non-irrigated land

Component	Date	Previous day's salt load (mg)	Salt input (mg)	Generated salt load (mg)	Percolated/ Baseflow salt load (mg)	Calculated current salt load (mg)	Simulated current salt load (mg)	Error (%)
Topsoil	09/04/95	16085289.81	2822982.34	57354.79	2121598.59	16844028.35	16844028.35	2.21E-14
	10/04/95	16844028.35	738574.00	55884.66	1851271.79	15787215.22	15787215.22	-1.18E-14
	11/04/95	15787215.22	102796.00	49223.82	1102430.26	14836804.78	14836804.78	-1.26E-14
Subsoil	09/04/95	26339019.30	2121598.59	55467.52	1277067.58	27239017.83	27239017.83	0.00E+00
	10/04/95	27239017.83	1851271.79	58847.14	1844888.75	27304248.01	27304248.01	1.36E-14
	11/04/95	27304248.01	1102430.26	58525.42	1751281.39	26713922.30	26713922.30	-1.39E-14
Groundwater	09/04/95	58423586.14	1277067.58	80043.85	932578.88	58848118.69	58848118.69	0.00E+00
	10/04/95	58848118.69	1844888.75	82517.21	948098.18	59827426.47	59827426.47	0.00E+00
	11/04/95	59827426.47	1751281.39	84828.09	961951.16	60701584.79	60701584.79	-1.23E-14

Table 6.4 Mass balance for code validation of subsurface salt movement processes in irrigated land

Component	Date	Previous day's salt load (mg)	Salt input (mg)	Generated salt load (mg)	Percolated/ Baseflow salt load (mg)	Calculated current salt load (mg)	Simulated current salt load (mg)	Error (%)
Topsoil	09/04/95	3433643113.07	18996567.25	54315547.83	28707284.68	3478247943.46	3478247943.47	-2.88E-10
	10/04/95	3478247943.46	11887930.01	54790044.42	39045159.05	3505880758.85	3505880758.84	2.85E-10
	11/04/95	3505880758.85	1676000.00	53885607.92	20438115.81	3541004250.96	3541004250.96	0.00E+00
Groundwater	09/04/95	1900848972.32	28707284.68	26075587.33	39112636.89	1916519207.44	1916519207.44	1.24E-14
	10/04/95	1916519207.44	39045159.05	26149707.83	39634281.49	1942079792.83	1942079792.83	0.00E+00
	11/04/95	1942079792.83	20438115.81	25928168.40	39768921.54	1948677155.50	1948677155.50	0.00E+00

6.5.2 Code validation of surface salt movement processes

The salt load associated with runoff water from irrigated and non-irrigated lands comprises salt load from baseflow and quickflow. Therefore, the "Calculated runoff salt load" column shown on Table 6.5 is computed as the sum of the baseflow salt load and quickflow salt load columns. This calculated salt load on a particular day is compared against the simulated output from the model. The "Error" column is then determined as the percentage difference between the runoff salt load as calculated on a spreadsheet and that simulated by the model. The result from this comparison shows that the algorithms involved in runoff salinity and salt load computations are yielding the required results with only minor errors. These minor errors are attributed to rounding errors.

Table 6.5 Mass balance for code validation of surface salt movement processes

Component	Date	Baseflow salt load (mg)	Quickflow salt load (mg)	Calculated runoff salt load (mg)	Simulated runoff salt load (mg)	Error (%)
Non-irrigated land	09/04/1995	932578.88	135068.07	1067646.95	1067646.95	0.00E+00
	10/04/1995	948098.18	94547.65	1042645.83	1042645.83	1.12E-14
	11/04/1995	961951.16	66183.35	1028134.51	1028134.51	0.00E+00
Irrigated land	09/04/1995	39112636.89	2548432.75	41661069.64	41661069.64	0.00E+00
	10/04/1995	39634281.49	222069.99	39856351.48	39856351.47	2.51E-08
	11/04/1995	39768921.54	0.00	39768921.54	39768921.54	0.00E+00

6.5.3 Code validation of reservoir salt budgeting processes

The major sources of salt input to an internal reservoir system accounted in *ACRUSalinity* are:

- runoff salt load from irrigated lands
- runoff salt load from non-irrigated lands
- runoff salt load from adjunct impervious areas and
- salt input through wet atmospheric deposition (salt load associated with the rain falling on the surface of the reservoir).

Similarly, the total salt outflow from a reservoir system comprises salt load associated with:

- seepage water
- overflow from the reservoir
- domestic or irrigation water abstracted from the reservoir and
- legal flow (normal) flow release.

The current salt load stored in the reservoir is calculated from considerations of the total inflow, total outflow and salt load stored in the reservoir at the end of the previous time step as:

calculated current salt load = previous day's salt load + total inflow – total outflow

The calculated current salt load is then compared against the simulated current salt load. The error value which is calculated as the percentage difference of the calculated and simulated current salt load is found to be minor. This minor difference shown on the "Error" column of Table 6.6 is due to rounding errors. Therefore, the algorithms describing the reservoir salt budget are performing the required tasks almost perfectly.

Table 6.6 Mass balance for code validation of reservoir salt budgeting processes

Reservoir inflow and outflow components		**Date**				
		07/04/1995	08/04/1995	09/04/1995	10/04/1995	11/04/1995
Salt inflow sources	irrigated	39050607.60	39111977.90	41661069.60	39856351.50	39768921.50
	non-irrigated	223842940.99	222263205.68	237597563.92	249456786.95	257730309.21
	rainfall	0.00	44400000.00	69264000.00	39072000.00	5683200.00
	impervious	0.00	39.35	63.09	34.26	2.37
	total salt inflow (mg)	262893548.61	305775222.92	348522696.66	328385172.68	303182433.12
salt outflow	seepage	1012.14	1056.84	1023.14	926.58	897.88
	overflow	0.00	413370181.63	850371375.03	456820732.84	115589219.49
	abstraction	33738035.34	35228150.71	34104644.47	30886105.40	29929333.62
	legal flow	1012.14	0.00	0.00	0.00	0.00
	total salt outflow (mg)	33740059.62	448599389.18	884477042.64	487707764.82	145519450.99
Previous day's salt load (mg)		5592810179.80	5821963668.80	5679139502.53	5143185156.54	4983862564.40
Calculated current salt load (mg)		5821963668.79	5679139502.54	5143185156.55	4983862564.40	5141525546.53
Simulated current salt load (mg)		5821963669.00	5679139503.00	5143185157.00	4983862564.00	5141525547.00
Error (%)		1.43937E-10	-1.5921E-10	-1.07398E-10	7.85119E-11	-1.29895E-10

6.5.4 Code validation of channel salt movement and distributed hydrosalinity modeling processes

In the presence of an internal dam the salt load associated with runoff from non-irrigated land and adjunct impervious areas of a sub-catchment is allocated to an internal dam and a channel reach. On the other hand, if no reservoir exists in the sub-catchment, or if it is situated at the sub-catchment's outlet, the total salt load associated with the runoff water from the sub-catchment is allocated to a channel reach. In the previous section's mass balance computation for a reservoir salt budget an internal dam was considered and in this case an external dam will be considered.

For the purpose of this code validation of channel and distributed hydrosalinity modelling processes, a simple catchment composed of four sub-catchments with one external dam situated at the outlet of Sub-catchment 3 is used. Layout of the sub-catchments and the direction of water flow and salt transport between the sub-catchments are shown in Figure 6.8.

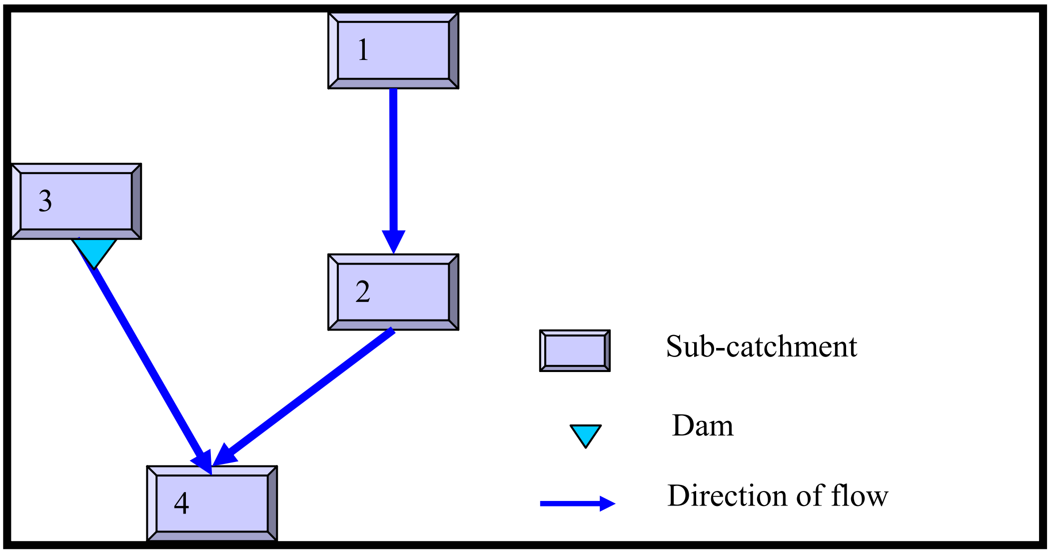


Figure 6.8 Layout and direction of salt transport for the catchment used in code validation of channel and distributed hydrosalinity modelling processes

On each sub-catchment the sources of salt input to a channel reach are:

- salt load associated with runoff water from adjunct impervious areas
- salt load associated with runoff water from non-irrigated lands
- salt load associated with runoff water from irrigated lands and
- salt load transported from upstream reaches, in the case of distributed hydrosalinity modeling.

No channel reach salt storage is assumed in *ACRUSalinity*. Therefore, on a particular day, the total salt load that enters the channel reach is transported to a destination reach on the same day. Thus, the total salt load at the river (channel) reach of Sub-catchment 2 (River_2) is calculated as the sum total of:

- streamflow salt load from river reach 1 (River_1)
- runoff salt load from adjunct impervious area in Sub-catchment 2
- runoff salt load from irrigated land in Sub-catchment 2 and
- runoff salt load from non-irrigated land in Sub-catchment 2.

Based on configuration of the four sub-catchments used for this purpose (Figure 6.8), the salt load from River_2 is transported to River_4. Similarly, the salt load associated with the total outflow from the external reservoir of Sub-catchment 3 (Dam_3) is allocated to River_4. Therefore, the calculated total salt load at River_4 in Table 6.7 is computed from the sum total of:

- salt load from River_2
- salt load from Dam_3
- salt load associated with runoff water from adjunct impervious area of Sub-catchment 4
- salt load associated with runoff water from irrigated lands of Sub-catchment 4, and
- salt load associated with runoff water from non-irrigated land of Sub-catchment 4.

The calculated total salt load at river reaches 2 and 4 are compared against the simulated values on these reaches. As shown on the "Error" column of Table 6.7, only minor rounding errors can be noticed. This reveals that the algorithms describing channel salt movement and distributed hydrosalinity modelling processes, except for the minor rounding errors, are also considered free from coding error and are performing the tasks for which they are intended.

Table 6.7 Mass balance in mg for code validation of channel and distributed hydrosalinity modelling processes

Component		Date		
		28-Dec	29-Dec	30-Dec
Total salt load at River_1		51466.7	55904.8	51561.1
Sub-catchment 2	Adjunct impervious area	0.0	1942228.5	303144.0
	Irrigated land	0.0	0.0	0.0
	Non-irrigated land	19634302.6	19684233.0	19562181.3
	Calculated total salt load at River_2	19685769.3	21682366.3	19916886.4
	Simulated total salt load at River_2	19685769.3	21682366.3	19916886.4
	Error (%)	3.97E-13	-8.59E-14	-2.24E-13
Outflow salt load from Dam_3		1745659.2	1753324.9	1707290.0
Sub-catchment 4	Adjunct impervious area	0.0	20457862.4	3206056.8
	Irrigated land	0.0	0.0	0.0
	Non-irrigated land	210476751.0	242962956.0	236110333.0
	Calculated total salt load at River_4	231908179.4	286856509.0	260940567.0
	Simulated total salt load at River_4	231908179.4	286856509.0	260940567.0
	Error (%)	1.28509E-13	-8.3114E-14	-2.3984E-13

6.6 Verification Against Observed Data

Discrepancies between observed and simulated responses of a system can be the manifestation of errors in the mathematical model. Simulation results are often less accurate than desired due to uncertainty in the input data provided to the model as well as uncertainties in the modelled processes (Rossouw and Kamish, 2001). According to Konikow (2002), in applying hydrological models to field problems, there are three sources of errors.

- One source consists of conceptual errors, i.e., theoretical misconceptions about the basic processes that are incorporated in the model. Conceptual errors include both neglecting relevant processes as well as representing inappropriate processes.
- A second source of error involves numerical errors arising in the equation-solving algorithm.
- A third source of error arises from uncertainties and inadequacies in the input of data that reflect our inability to describe comprehensively and uniquely attributes of the system.

In most model applications conceptualisation problems and uncertainties concerning data are the most common sources of error (Konikow, 2002). *ACRUSalinity* is validated for the second source of error (coding error) as described in the previous section. This section, therefore, presents the assessment made on the combined effects of the first source of error (conceptual error) and the third source of error (data uncertainty). A sensitivity analysis is also undertaken (Chapter 7), in order to assess the effects of data uncertainty and errors on module outputs.

6.6.1 Observed daily flow and TDS concentration

Observed data from the Mkomazi Catchment were used for data patching and comparison of simulated model outputs. The observed data used for these purposes include daily flow and its TDS concentration value. Daily streamflow depth for the U1H005 gauging weir, where the Upper Mkomazi Catchment drains, was obtained from DWAF. Similarly, the streamflow salinity data for this station is obtained from the "Water Quality on Disc" CD-ROM (CSIR, 2002). This disc gives access, on a PC, to many of the macro-chemical water quality data-bases for the area, such as EC, TDS, PH and most base elements. Streamflow TDS concentration grab samples collected on a weekly basis from January 1986 to December 1987 are used for calibration (1986) and verification (1987) purposes. This period is chosen because it has relatively few missing records compared to data records of the remaining years for the station.

6.6.2 Observed data conversion and patching

The salinity data, in mg/l, for the calibration and verification periods is based on weekly grab samples. Hence, conversion to daily values was necessary so as to be used for comparison with the daily model output. Therefore, filling of missing values and subsequent conversion to daily data are done in two steps. The first step involved patching missing TDS values from the EC record, if the EC value was available for the given day. The second step involved data patching using the TDSGEN program which has been developed by Ninham Shand Consulting Engineers. This program infills missing data based on flow-TDS relationships recorded in the area.

The patching of missing TDS values from EC values was based on a regression equation established using observed TDS and EC values. The relationship between TDS (mg/l) and EC (ms/m) as recorded at gauge U1H005 is plotted in Figure 6.9. The linear regression analysis yielded the following relationship with coefficient of determination (R^2) of 0.79:

$$TDS = 6.388 * EC + 8.256 \qquad (6.1)$$

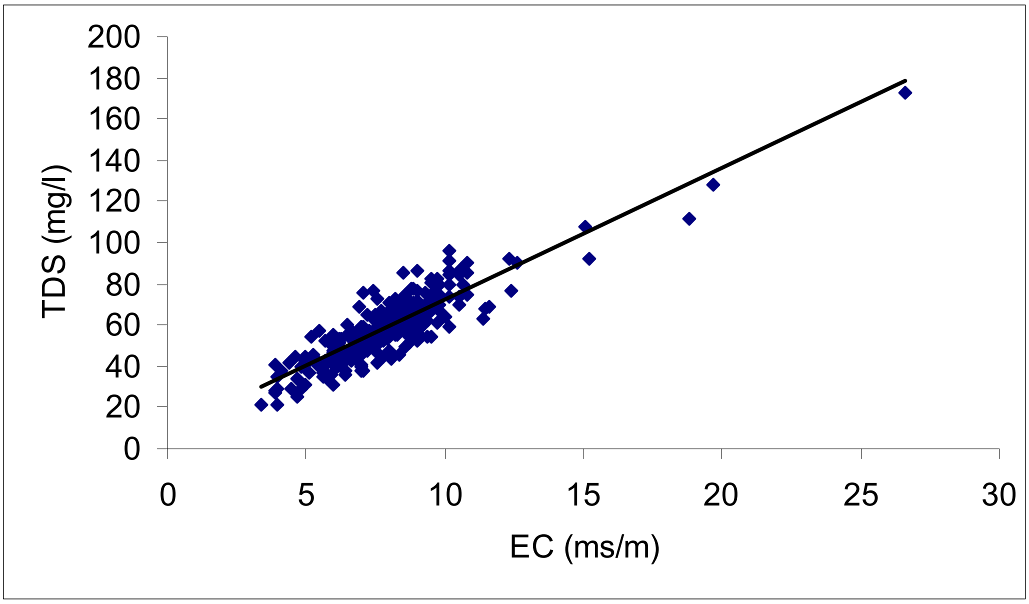


Figure 6.9 TDS versus EC relationship as recorded at U1H005 (Camden)

First, available conductivity measurements for the area are converted to TDS values by using Equation 6.1. Then, if on a particular day, a recorded TDS value does not exist while a conductivity value does, the converted EC value is used to fill the missing TDS value. However, if neither TDS nor EC values are recorded on the particular day the missing values are infilled by use of the TDSGEN program.

6.6.3 Calibration of the *ACRUSalinity* module

According to Konikow (2002) model calibration may be viewed as an evolutionary process in which successive adjustments and modifications to the model are made based on the results of previous simulations. The modeller decides when sufficient adjustments have been made to the representation of parameters and processes and at some time accepts the model as being adequate (or perhaps rejects the model as being inadequate and seeks alternative approaches). This decision is often based on a mix of subjective and objective criteria. Some of these criteria include the visual fit between plots of time series of simulated and observed salt concentrations and through comparison of statistical outputs such as means, standard deviations and correlation coefficients of simulated and observed values. In general the objective of model calibration is to minimise differences between the observed data and simulated values. Usually the model is considered calibrated when it reproduces historical data within some acceptable level of accuracy. The acceptable level is determined subjectively (Konikow, 2002).

As mentioned in Section 6.3.2.3, the attempt to derive values of the salt uptake rate constant (k) through fitting a regression equation to an observed streamflow TDS concentration data was not successful owing to the lack of a daily soil moisture salinity data. Hence, an attempt was made to obtain a representative rate constant (k) and equilibrium (C_e) value for the area through calibration of the module. This was achieved by changing these values in an attempt to optimise the module predictions of the streamflow salinity against the observed data. The graphical and statistical methods employed for the calibration purpose are outlined below.

6.6.3.1 Time series and percentile curves

Both time series and percentile curves are used to estimate values of the rate constant and equilibrium parameters that yield the best fit between observed and simulated streamflow TDS concentration values. Figures 6.10 and 6.11 show the time series and percentile curves respectively for the calibration period (from 01 January, 1986 to 31 December, 1986). From the various calibration trials undertaken to obtain a representative uptake rate constant (k) and an equilibrium (C_e) values for the Upper Mkomazi Catchment, the best fit (Figures 6.10 and 6.11) is attained at a k value of 4.5E-5 and C_e value of 3000 mg/l. During the calibration trials constant values of k and C_e parameters are used in all sub-catchments.

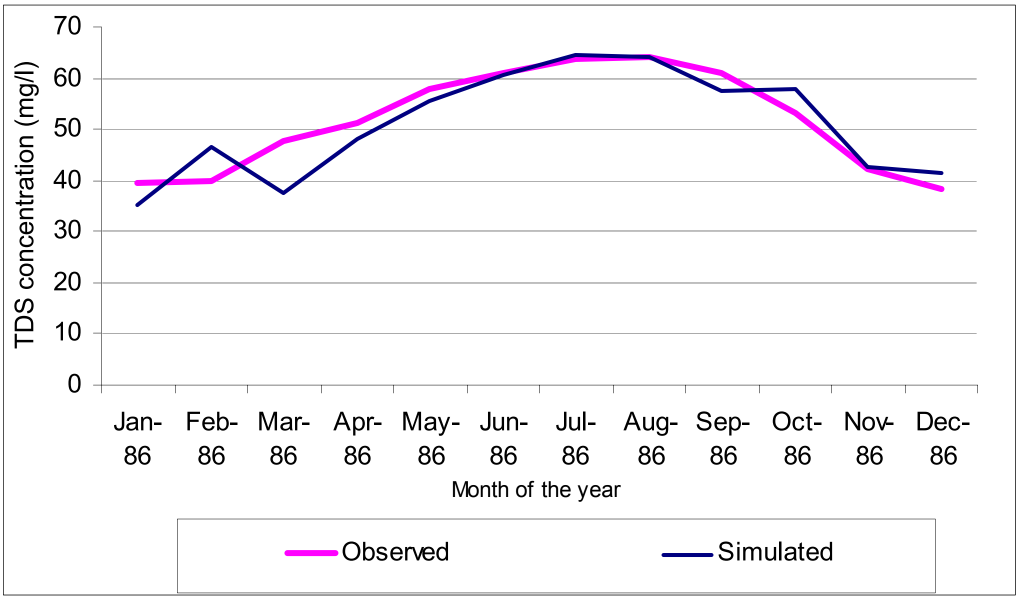


Figure 6.10 Monthly means of daily observed and simulated streamflow TDS concentration at Camden for the calibration period (U1H005)

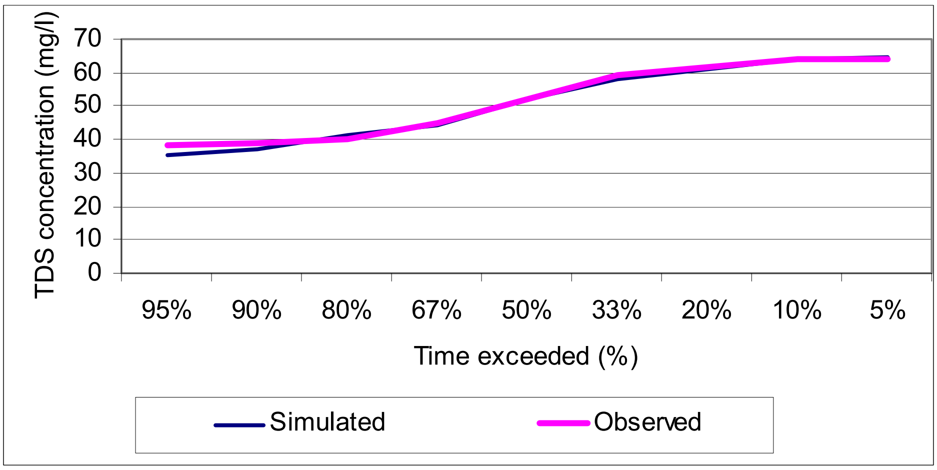


Figure 6.11 Percentile curves for observed and simulated monthly means of daily streamflow TDS concentration at Camden for the calibration period (U1H005)

6.6.3.2 Statistical analysis

According to Schulze *et al.* (1995), the general aim of a good simulation is a one to one correspondence between simulated and observed values, with a high correlation, a minimum symmetric error and the conservation of means, deviations and other statistics. The wide range of goodness-of-fit statistics comparing observed and simulated values can be categorised into conservation statistics and regression statistics. The conservation statistics that include mean, standard deviation and skewness coefficient are employed in this dissertation for comparison of observed and simulated values. A summary of these statistics for the calibration period are shown in Table 6.8. Similarly, regression statistics for comparison of observed and simulated values including correlation coefficient, coefficient of determination, slope as well as y-intercept for the scatter plot of observed versus simulated values are also given in Table 6.9.

The general aim during the procedure with regard to the conservation statistics was to minimise:

- the percentage difference between means of observed and simulated values
- the percentage difference in standard deviation, i.e. in minimising the difference in dispersion of the observed and simulated data about their mean values and
- the percentage difference in skewness coefficient, i.e. the symmetry of the observed and simulated values.

Conversely, the aim with regard to the regression statistics used was to:

- maintain a slope as close as possible to 1.0 since a slope value greater than one indicates over-simulation whereas a slope value less than 1.0 indicates under-simulation (Schulze *et al.*, 1995)
- minimise the base constant (y-intercept) to zero
- maximise the correlation coefficient to unity and
- maximise the coefficient of determination to unity.

Table 6.8 Conservation statistics of streamflow salinity at Camden (U1H005)

Statistical parameter	Observed	Simulated	Difference %
Mean (mg/l)	51.67	51.00	-1.30
Standard deviation	9.96	10.30	3.41
Skewness Coefficient	-0.12	-0.14	16.67

Table 6.9 Regression statistics of streamflow salinity at Camden (U1H005)

Statistical parameter	Value
Slope	0.94
Base constant (y-intercept)	2.65
Correlation coefficient	0.90
Coefficient of determination	0.82

As it can be seen from the time series and percentile curves, the simulated streamflow TDS concentration has shown good fit with the observed values at U1H005 when a salt uptake rate constant of 4.5E-5 and an equilibrium value of 3000 mg/l are used. This is also confirmed from the statistical analysis shown in Tables 6.8 and 6.9. Therefore, these values are taken as representative values for k and C_e parameters in the catchment.

6.6.4 Verification result and discussion

The uptake rate constant (k) and the equilibrium values as determined from the calibration result are used as input in simulating streamflow TDS concentration for the verification period (January to December, 1987). Both graphical and statistical methods are then used to evaluate the module performance using the same criteria as considered for calibration.

6.6.4.1 Time series and percentile curves

The daily simulated TDS concentration values and the observed values from the weekly samples are plotted in the same graph (Figure 6.12). From Figure 6.12 it can be seen that the simulated values follow the observed seasonal fluctuations remarkably well. Similarly, the monthly mean of daily observed TDS concentrations which are patched from the weekly grab samples are plotted in the same graph with the simulated values as shown in Figure 6.13. From Figure 6.13 it can be seen that the simulated TDS concentration follow the observed seasonal fluctuations remarkably well. However, the monthly mean of daily simulated TDS concentration values, especially from April to August of the verification year (1987), have slightly exceeded the observed streamflow salinity values. On the other hand, the simulated streamflow TDS concentration values for the period of October to December have shown very good fits with the observed values (Figure 6.13).

Figure 6.14 shows observed and simulated percentile curves of the daily streamflow TDS concentration at Camden for the verification period. In general, the percentile curve for simulated values has followed the trend of observed streamflow TDS concentration curve very well. However, the graph shows an overall slight over-simulation of streamflow TDS concentrations, especially for those with relatively higher values (values that would be exceeded in less than 50 % of the time).

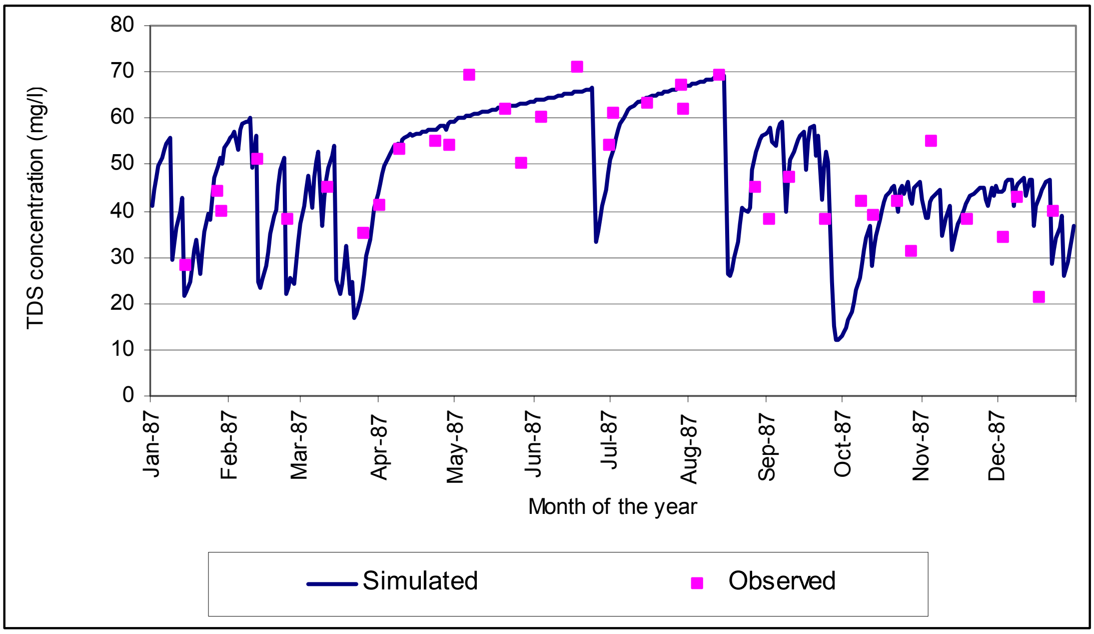


Figure 6.12 Observed (weekly grab of samples) and daily simulated streamflow TDS concentration values at Camden (U1H005)

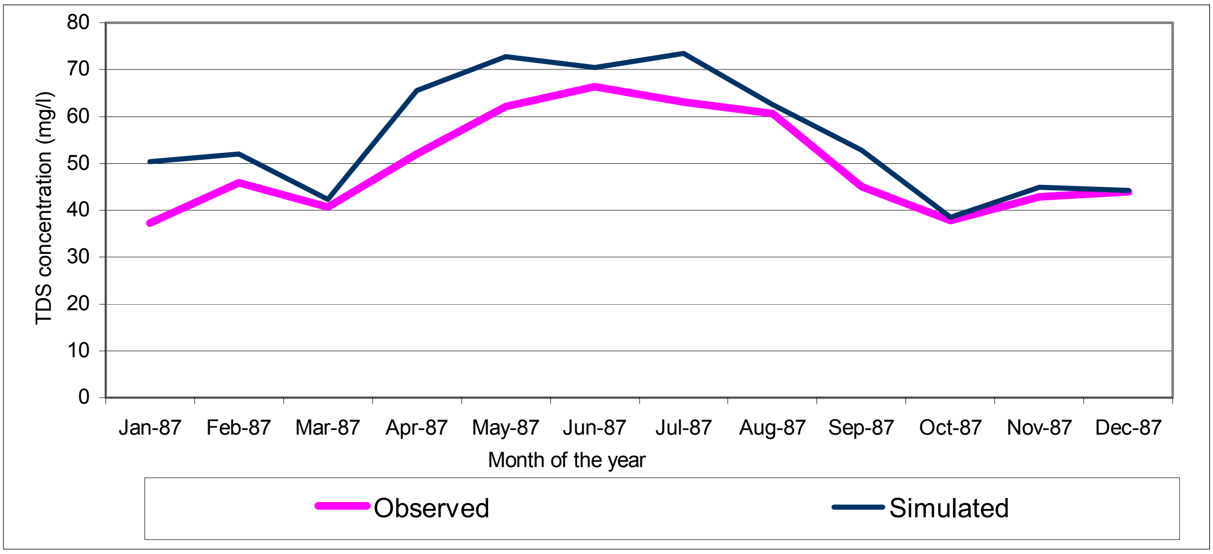


Figure 6.13 Monthly means of daily observed (patched with TDSGEN) and simulated streamflow TDS concentration values at Camden for the verification period (U1H005)

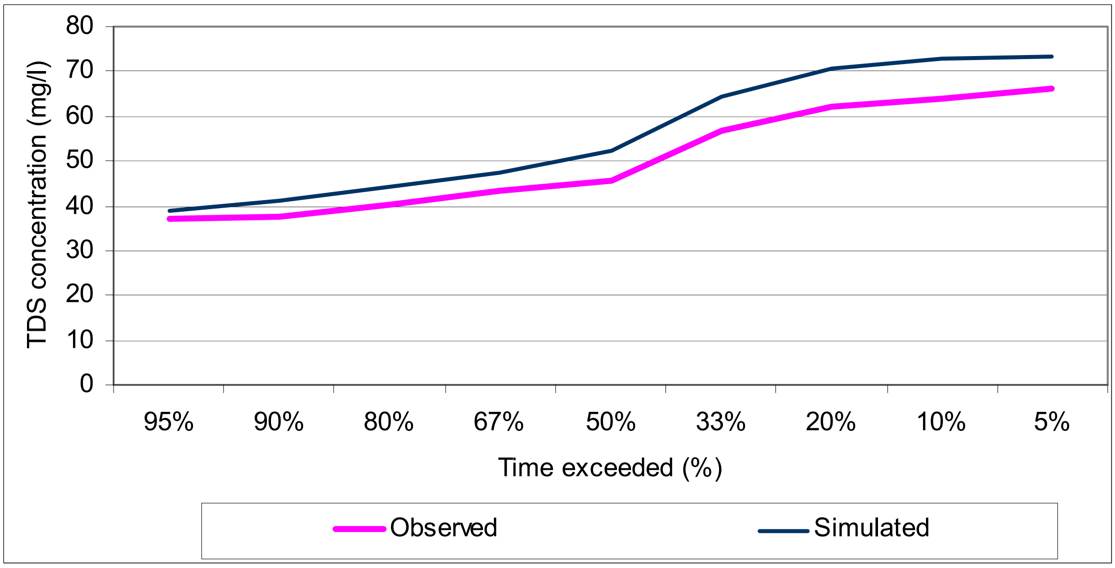


Figure 6.14 Percentile curves of observed (patched with TDSGEN) and simulated TDS concentration values at Camden for the verification period (U1H005)

6.6.4.2 Statistical analysis

Both conservation and regression statistics are used to compare the simulated and observed streamflow TDS concentrations. Results from the statistical analysis are shown in Tables 6.10

and 6.11. In both tables the “Daily” Column refers to value of the statistical parameter determined using daily simulated values and daily observed values which are patched using the TDSGEN program from the weekly grab of samples, whereas the “Weekly” Column refers to value of the statistical parameter calculated using only the weekly grab of samples and the simulated values for the particular day. In general the conservation and regression statistics show a fair ability of the hydrosalinity processes encoded in *ACRUSalinity* to mimic the natural processes taking place in the catchment.

- The conservation statistics, save for the skewness coefficient, do not indicate high divergence between observed and simulated values. The high difference observed between the skewness coefficients, however, reveals a considerable difference in the symmetry of the observed and simulated salinity distributions.

- The regression statistics show a very good fit with:

    - the slope showing a slight over-simulation of the model,
    - the Y-intercept having a value close to 0, showing a slight over-simulation, and
    - the correlation coefficient and coefficient of determination showing a high degree of association between observed and simulated values.

Table 6.10 Conservation statistics of streamflow TDS concentration at Camden (U1H005)

Statistical parameter	**Observed**		**Simulated**		**Difference %**	
	Daily	**Weekly**	**Daily**	**Weekly**	**Daily**	**Weekly**
Mean (mg/l)	49.81	48.12	55.82	48.33	12.07	0.44
Standard deviation	10.57	10.18	12.57	12.49	18.92	22.69
Skewness Coefficient	0.45	0.42	0.21	-0.31	-53.33	173.81

Table 6.11 Regression statistics of streamflow TDS concentration at Camden (U1H005)

Statistical parameter	**Value**	
	Daily	**Weekly**
Slope	1.11	0.97
Base constant (y-intercept)	0.33	1.52
Correlation coefficient	0.92	0.79
Coefficient of determination	0.87	0.63

6.7 Conclusions

This chapter has discussed the code validation and verification of the hydrosalinity module of *ACRU*. The code validation which was undertaken based on the principle of mass conservation has shown that the major algorithms of the new module are free of errors emanating from incorrect computer coding, except for minor rounding errors. Similarly, the verification undertaken to evaluate how this module performs under field conditions through comparison of model simulation against observed data has yielded good result when taking into account the data limitations for some of the hydrosalinity input parameters for the Mkomazi Catchment, and considering the complex nature of actual hydrosalinity processes, as they involve geochemical processes in addition to all of the other processes influencing water quantity.

The next chapter reviews the various sensitivity tests undertaken in this project in order to examine model response to changes in values of the main input parameters of *ACRUSalinity* and a case study in the Mkomazi Catchment to demonstrate some potential applications of the module.