3. REVIEW OF HYDROSALINITY MODELLING APPROACHES

A hydrosalinity model is a mathematical description of the fate and transport of water and chemicals in the soil (Moolman, 1993). Addiscot and Wagenet (1985) suggest that, before making further attempts to model solute movement, it is important to place existing modelling approaches in perspective, comparing and classifying them on several levels, indicating those cases for which they were intended to be applied, and discussing the accuracy of model predictions under field situations in which solute transport models have been tested. This helps for future modelling efforts to proceed with a clear recognition of modelling approaches as a function of the modeller's purpose, realising in the process the inherent strengths and weaknesses of each method. Therefore, this chapter will attempt to review the basic types of water quality and quantity models followed by a review of processes involved in hydrosalinity with special emphasis on soil salt balance and movement and the commonly used modelling approaches to describe these processes.

3.1 Types of Hydrosalinity Models

Various researchers have attempted to classify hydrosalinity models. However, most of the models fall into one of the types described in the following sections. *ACRUSalinity* is a hydrosalinity module, i.e. it is premised around the dominance of the hydrological "forcing" processes, which links the fate of salt to the fate of water. This section, therefore, classifies hydrosalinity models mainly based on physical processes rather than chemical processes such as sorption, dissolution and precipitation. According to Kienzle *et al.* (1997), hydrological and water quality modelling are commonly performed using one or more of the following four different modelling approaches.

3.1.1 Calibration and parameter optimizing models

These are models in which parameters of the model are adjusted to enable the model output to match observations as closely as possible. The major drawbacks of these models are that they are data demanding (for the calibration procedure) and that parameters are identified for a particular catchment. This makes parameter transfers to ungauged catchments problematic and speculative.

3.1.2 Parametric models

These are so-called “grey box” models which are sometimes referred to as conceptual models. Parametric models represent a partial understanding of processes. However, the system’s spatial heterogeneity (e.g. of soils, vegetation, terrain) is not taken into account explicitly because inputs (and hence outputs) are spatially averaged (lumped). Consequently, hydrological processes and their variability are integrated in such a way that their parameter expressions are often indices rather than having strictly physically meaningful values. Thus an underlying problem in using parametric models is that these models use parameters to represent catchments as a whole, whereas data on catchment characteristics are collected at multiple field locations and are difficult to transform into one measure of collective impact (Song and James, 1992).

3.1.3 Stochastic models

These are so-called “black-box” models, in which inputs (e.g. rainfall) are transformed to outputs (e.g. runoff) with little or no understanding of the processes involved in the transformation. This type of model relies on historical records of both input and output variables that are a representative sample over time.

According to Quilez *et al.* (1992), an improvement has recently been observed on simple regression models with the incorporation of random noise theory for application in modelling water quality variables. In most of these regression based water quality models, streamflow has been considered as the most important driving variable. In general, water quality variables, and in particular salinity, are known to be related to streamflow. Regression models for this relation have been proposed and applied in different basins. These models do not consider the temporal and dynamic relationships between the primary variables. However, the random noise theory based models try to introduce a stochastic (noise) component into the model, based on the fact that water quality variables do not behave in a completely deterministic manner with respect to streamflow. This approach was employed to study the flow-salinity relationships on the Ebro River Basin in Spain (Quilez *et al.,* 1992) and by Herold and Eeden (2001) in an effort to relate river water quality and diffuse loads to a range of land uses in South Africa.

The empirically developed and commonly used function to describe flow-salinity relationship assumes, among other conditions, that mixing is complete and there is no hysterics in the flow salinity relationship. This expression is commonly described as: $EC = aQ^b$, where EC is the electrical conductivity, Q is the discharge, a and b are regression coefficients. This regression equation is referred to as a dilution model (Walling and Webb, 1986).

Transfer function-noise models are similar to regression models such as the above named dilution model, the main difference being the addition of the noise component. In order to account the stochastic nature of water quality variables, the above equation is, in most cases, reduced to a linear form by taking natural logarithms. Random noise is then added to the regressed values for each day. The random noise is computed through a series of steps. Herold and Eeden (2001), for example, have used a random number generator to provide a random number for each day of the record. These random numbers were then normalised in order to conform to a normal distribution. The normalised random number for each day simulated is then multiplied by the standard error for the observed data set.

In general, according to Quilez *et al.* (1992), transfer function-noise approach models represent an improvement over simple regression models in terms of higher explained variance, and they represent the advantage of having a related flow series. They also represent marked improvement over classical regression models for cases in which the relation between salinity and flow is not instantaneous. The effect of not including random noise to the regression line is reflected in the research results of Herold and Eeden (2001), where the use of a regression line alone, with no allowance for the observed variance about the regression, has affected the results very severely, with the result that the peak values were much too low.

3.1.4 Deterministic, physically conceptually based models

These belong to the group of near "white box" models, in which the behaviour of the hydrological system is described in terms of mathematical relationships which represent the interactions and linkages of the various components of spatially and temporally varying hydrological processes. Deterministic hydrosalinity models may further be classified to mechanistic and functional models.

For the purpose of this dissertation these models are more important than the other types of hydrosalinity models. Therefore, the following sections will attempt to review with more detail the two subdivisions of deterministic models, *viz.* mechanistic and functional models.

3.1.4.1 Mechanistic models

Physically based flow and transport models use as a basis, continuum mechanics theory for the way in which substances migrate. Since these models attempt to represent the coupled flow system that is operating, the mathematical description also usually results in a system of coupled partial differential equations (Connel *et al.*, 2001).

Mechanistic models are broadly characterised by the use of rate parameters and their use as research tools. The use of rate parameters for solute movement combines the description of several transport processes (Addiscot and Wagenet, 1985). It first defines the instantaneous flux of water content in terms of the product of a hydraulic gradient and a rate parameter, *viz.* hydraulic conductivity (based on Darcy's Law), and then defines the flux of solute concentration in terms of two other rate processes, *viz.* convection and diffusion. Thus, they describe the fundamental mechanisms of the physical processes involved in the leaching of solutes (Hall, 1993). Mechanistic models are often described as research (rather than operational) tools, in that they are developed to aid the testing of hypotheses and the exposure of areas of incomplete understanding. Although mechanistic models have a solid theoretical basis and have been widely used, when compared to the other soil-water-solute models their predictions can be misleading unless their inputs are well characterised with respect to variability. Thus, they require a detailed knowledge of the soil's pore-size distribution and hydraulic properties. Moreover, it is not yet established that they necessarily give more reliable or more accurate simulations of water and solute movement than the simpler, more functional models (Addiscot and Wagenet, 1985).

3.1.4.2 Functional models

The term functional is used for models that incorporate simplified treatments of solute and water flows and make no claim to fundamentality. They require less input and computer expertise for their use (Addiscott and Wagenet, 1985). According to Hall (1993), functional models use a simplified approach to describe water flow and solute transport and generally divide the soil profile into layers, with water and solute being passed from one layer to the next, usually on a daily basis. The amount of water passing through each layer depends on the pore volume available for mobile water, which is defined by the moisture release characteristics of the soil. Another important characteristic of functional models is their use of capacity parameters such as the volumetric water content at drained upper limit (DUL), instead of rate parameters. Thus, they define changes (rather than rates of changes) in amounts of solute and water content. Furthermore, unlike mechanistic models which are driven by rates, functional models are usually driven by the amounts of rainfall, evaporation or irrigation and only consider rates indirectly.

Functional models are generally used for management purposes. They are less rigorous than mechanistic models in terms of describing the processes involved in release, transportation, and deposition of salts. However, their input requirements are simpler and more readily available for a wider range of soils. Their reliance on capacity-type soil water inputs enables them to avoid the spatial variability problems associated with the rate inputs, but could result in failure to simulate variation in leaching that might be of practical importance (Addiscot and Wagenet, 1985). The *ACRU* agrohydrological modelling system, for example, belongs to this group of hydrological models (Schulze, 2001).

The procedure followed by Kienzle *et al.* (1997) classified hydrology and water quality models into four classes. In another classification by Addiscott and Wagenet (1985), hydrosalinity models are broadly classified as deterministic and stochastic models (Figure 3.1). The general concepts behind these models are similar to those in the preceding classification. Deterministic models presume that a system, or process, operates such that the occurrence of a given set of events leads to a uniquely definable outcome, whereas stochastic models presuppose that the outcome is uncertain and are structured to account for this uncertainty. Addiscott and Wagenet (1985) also classify deterministic models into mechanistic and functional models that are recognised by the characteristics described in the preceding sections. They also make a distinction between rate and capacity, as well as research and management models, which again corresponds broadly to the distinctions between mechanistic and functional models.

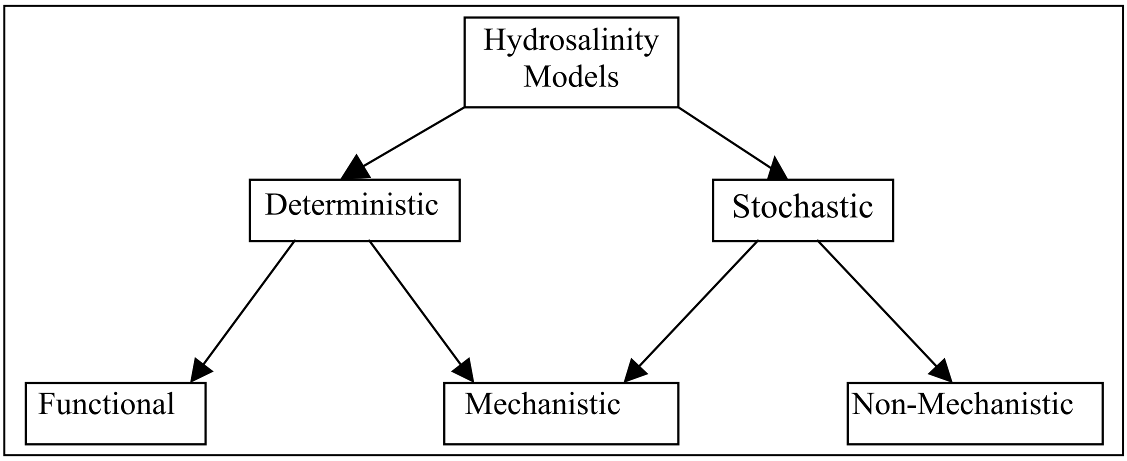


Figure 3.1 Classification of hydrosalinity models according to Addiscot and Wagenet (1985)

3.2 Classification of Hydrosalinity Models Commonly Used in South Africa

Some of the hydrosalinity models commonly used in South Africa are shown in Table 3.1, according to a classification by Jonker (1995). The classification is based on Addiscott and Wagenet's (1985) procedure.

Table 3.1 Classification of some hydrosalinity models used in South Africa according to Addiscott and Wagenet's classification procedure (after Jonker, 1995)

Model	Deterministic/ Stochastic	Functional/ Mechanistic	Research/ Management	Lumped or Distributed parameter
NACL (Herold, 1981)	Deterministic	Functional	Management	Lumped
FLOSAL (Hall and Du Plessis, 1981)	Deterministic	Functional	Research	Lumped
IRRIS (Forster, 1987)	Deterministic	Functional	Management	Lumped
LEACHM (Wagenet and Hutson, 1989)	Deterministic	Mechanistic	Research	Lumped
DISA (NSI, 1990)	Deterministic	Functional	Research and Management	Lumped and Distributed

From Table 3.1 it can be noticed that most of the hydrosalinity models commonly used in South Africa are deterministic functional models. However, most of the models listed in the table are lumped models. Therefore, this calls the need for a distributed hydrosalinity model which is applicable in complex land use or larger catchments.

In the preceding sections an attempt was made to review the common types of water quantity and quality models in general and hydrosalinity models in particular. In the following sections some of the deterministic hydrosalinity modelling approaches are reviewed in more detail with special emphasis on describing the basic processes that influence salt balance and movement through the soil profile.

3.3 Mechanistic Modelling Approaches of Salt Balance and Movement in Soils

Despite the difficulties involved in obtaining the necessary soil, water and salt measurements required for mechanistic models, they are nevertheless widely used, especially for research purposes. The main salt transport and mixing mechanisms such as diffusion, dispersion and convection, as well as associated processes, are described below.

3.3.1 Diffusion

According to Leij and Genuchten (1999), solute molecules in a free solution possess random thermal motion which causes an exchange of molecules between adjacent volume elements. A net transfer of molecules of a solute species usually occurs when the concentration of the species differs in adjacent volume elements, i.e. more particles move from the elements with higher concentrations to those with lower concentrations than vice versa. The resulting process is referred to as diffusion. Diffusion is an important mechanism for the transport of solutes in the liquid phase in directions of low mean pore-water velocities with relatively little, or no, water flow. The maximum flux (J_{dif}) due to molecular diffusion has the dimension of mass per unit area per unit time ($ML^{-2}T^{-1}$) and it is usually expressed by Fick's first law which states that the transport of the substance in a space direction is proportional to the gradient of the concentration of this substance in that direction, with the proportionality factor being the coefficient of diffusion (Jolankai, 1997). This law, for one dimentional diffusion, yields:

$$J_{dif} = -\theta D_o \frac{\partial c}{\partial x} \tag{3.1}$$

where x is distance (L), θ is water content, c is the solute concentration and D_o is the coefficient of molecular diffusion for a free (or bulk) solution (L^2T^{-1}) whose value depends on properties of both the solute and solvent (Leij and Genuchten, 1999).

The path of diffusion becomes more tortuous when there is less water available to move through, which further reduces the actual values of D_0 (Herald, 1999). As the water content of a soil decreases, the cross-sectional area available for diffusion becomes smaller and the ions have to travel a longer distance to reach a given point. Other factors such as viscosity and anion exclusion become more influential as water content decreases (Herald, 1999). Therefore, to describe diffusion in a porous medium such as soil, the diffusivity in a free solution is typically adjusted to account for a reduced solution phase (a smaller cross-sectional area available for diffusion), and an increased path length. The macroscopic diffusive flux per unit area of soil can be written as (Leij and Genuchten, 1999):

$$J_{dif} = -\theta D_* \frac{\partial c}{\partial x} \tag{3.2}$$

where D_* is the coefficient of molecular, or ionic, diffusion for the liquid phase of the soil. The diffusion coefficients for the soil liquid and a free liquid are related by $D_* = D_0/(L_*/L)^2$, where L_* is the actual path length for diffusion in the soil (which depends on θ), L is the (straight) length of the soil and L_*/L is the tortuosity.

3.3.2 Mechanical dispersion

The macroscopic convective transport of a solute is usually described by an equation that takes into account two modes of transport, *viz.* the average flow velocity and mechanical dispersion (resulting from local variations in flow velocities). The mechanical dispersion component is similar to diffusion in the sense that there is a net movement of solute from zones of high concentration to zones of low concentration (Bresler, 1981).

Variation in water flow in a porous medium leads to mechanical dispersion. Several factors contribute to mechanical dispersion, and hence, to increased spreading. Initially steep concentration fronts will become smoother during movement along the main flow direction. Dispersion may occur as a consequence of one or more of the following factors (Wild, 1981; Leij and Genuchten, 1999):

- the development of a velocity profile in an individual pore, such that the highest velocity occurring in the center of the pore, and presumably little or no flow at the pore walls,
- different mean flow velocities in pores of different sizes,
- the mean water direction in the porous medium being different from the actual streamlines within individual pores, which differ in shape, size and orientation, and
- particles originating from different pores ending up in the same pore, and vice versa.

Although molecular diffusion and mechanical dispersion are different processes, the macroscopic solute flux due to mechanical dispersion is often conveniently expressed with Fick's first law of diffusion (Leij and Genuchten, 1999). For one dimensional dispersion in a uniform porous medium this leads to:

$$J_{dis} = -\theta D_{dis} \frac{\partial c}{\partial x} \tag{3.3}$$

where J_{dis} is the dispersive solute flux ($ML^{-2}T^{-1}$) and D_{dis} is the coefficient of mechanical dispersion ($L^{2}T^{-1}$). The dispersion coefficient (D_{dis}) is proportional to first power of the average velocity (Bresler, 1981), i.e. $D_{dis} = \lambda|V|$, where λ is the dispersivity and $|V|$ is the absolute value of the average flow velocity. The dispersivity is an intrinsic physical property of the porous medium and has unit of length (Herbert and Mary, 1982). Dispersion coefficients can be estimated with semi-empirical formulae or with the aid of *in situ* tracer measurements (Reichert *et al.*, 2001).

The macroscopic similarity between diffusion and mechanical dispersion enables both processes to be described with one coefficient of hydrodynamic dispersion. This practice is consistent with results from typical laboratory and field experiments, which do not distinguish between mechanical dispersion and molecular diffusion (Leij and Genuchten, 1999).

3.3.3 Convection and combined convective-diffusion transport

Solute transport is made up of two convective or mass flow components. In larger pores, turbulent flow dominates and fast convection occurs. On the other hand slow laminar transport occurs adjacent to particle surfaces and in micropores (Herald, 1999). In the case of conservative solutes no gains or losses and no solute-with-soil surface or solute-with-solute interactions occur. Under such circumstances the convective flow of solutes associated with water movement is expressed by $Jc = q.c$, where Jc = convective flux of solute, q = rate of volumetric water flow and c is solute concentration (Wild, 1981).

In the preceding discussion three types of solute transport mechanisms have been described, *viz.* molecular diffusion and the two modes of convective flow. However, these three components of solute transport occur simultaneously in natural soils (Bresler, 1981). Thus solute transport in soils has generally been described with the convection-dispersion equation. This equation incorporates two constitutive transport processes (Leij and Genuchten, 1999), *viz.* solute movement as a result of liquid flow, and spreading as a result of known and unknown processes such as diffusion and small-scale variations in water flow velocity.

An inherent assumption made by different modellers, in order to make their models simpler for the simulation of convective-diffusion transport of solutes is that the soil is an inert porous medium. In that case the total solute flux (Js) due to the joint effects of diffusion and convection can be described as (Bresler, 1981)

$$Js = -\theta D \frac{\partial c}{\partial x} + qc \tag{3.4}$$

where c is salt concentration in the soil solution, D is hydrodynamic dispersion coefficient, θ is volumetric water content, x is flow direction and q is volumetric water flux. However, water and solutes move at different rates through soil and may be acted upon, transformed or retarded during their movement through the soil (Herald, 1999). Therefore an expression for one-dimentional transient conditions should be derived from a consideration of continuity or mass conservation (Bresler, 1981). This states that the rate of change of solute within a given soil element must be equal to the difference between the amounts of solute that enter and leave that element. For the case of one dimensional vertical flow the following expression has been derived by equating the difference between outflow and inflow to the amount of salt that has accumulated in the soil element (Bresler, 1981; Runkel, 1998):

$$\frac{\partial(Q_a+\theta c)}{\partial t}=\frac{\partial}{\partial x}(\theta D\frac{\partial c}{\partial x})-\frac{\partial(qc)}{\partial x}+S \qquad (3.5)$$

where t is time, Q_a is the local concentration of solute in the adsorbed phase (meq.cm^{-3} soil), S is any solute loss (sink) or gain (source) due to salt uptake, sorption, precipitation or dissolution, and x is the vertical space co-ordinate (considered to be positive downward). S can be dealt through linear or nonlinear isotherms (Leij and Genuchten, 1999). The above equation is applicable for both reactive and non-reactive solutes, including the case when there is loss or gain of salt inside the flow system.

In general, the convection-dispersion equation (CDE) is the foundation upon which numerous mathematical analyses of solute transport in porous media have been based (Russo, 2002). Questions have, however, been raised regarding the applicability of the CDE at the field scale in which there are large variations in pore water velocities caused by spatial variability in soil hydraulic properties.

3.3.4 Miscible displacement

Miscible displacement experiments are important tools in the quantitative analysis of solute concentration changes in soils (Smettem, 1986). According to Bresler (1981), most works on miscible displacement phenomena are limited to steady state water flow with constant flow velocities and water contents. As such, these studies provide a means of determining hydrodynamic dispersion coefficients, evaluating macroscopic flow velocities and giving physical explanations for mixing phenomena that occur when salts flow through soils.

Miscible displacement phenomena in soils are illustrated by a classical experiment in which a solute is continuously introduced at the up-gradient end of a laboratory soil column (Herbert and Mary, 1982). When a salt-free soil solution is displaced through a column of soil by a solution containing an inert (non-reacting) solute of concentration C_0 at pore water velocity V and water content θ, the fraction of this solute in the effluent at time t can be designated as C/C_0, where C is solute concentration of the effluent. Plots of C/C_0 versus pore volumes of effluent are commonly called break-through curves, BTC (Figure 3.2). Pore volume refers to ratio of volume of effluent to volume of solution contained in the soil column.

The shape and development of the BTCs are very important to the understanding of solute behaviour when the solute percolates through porous media and when pore volume is set to unity as a reference (Matos *et al.*, 1999). It is then possible to derive important conclusions about the soil solute interactions simply by the position of the curves in relation to this reference. As to the physical explanation of the resulting different types of break-through curves, Bresler (1981) states that if piston displacement were operative, no mixing would occur between the displacing and displaced solutions and a vertical line would represent solute break through. A sigmoidal shape of break-through curve, on the other hand, indicates mixing (longitudinal dispersion) of the solution. Shifting of the curve to the left indicates exclusion from, or by-pass of, a significant portion of the soil solution. Displacement to the right indicates adsorption or retention of the solute by soil (Figure 3.2).

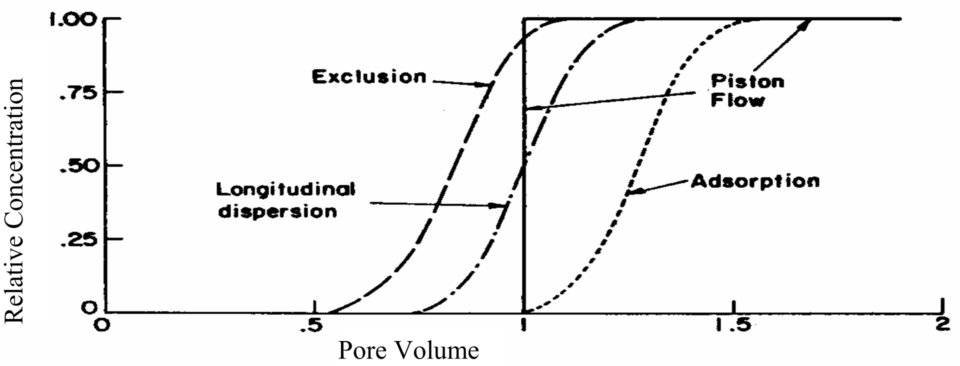


Figure 3.2 Schematic break-through curves for various miscible displacement conditions (after Bresler, 1981)

According to Lorentz (1986), break-through curves can be symmetrical or asymmetrical and can be influenced by other factors in addition to the governing soil-solute interaction mechanisms. Some of these factors affecting the shape of the BTC include soil particle and aggregate size, the ratio of micro- to macro-space volume and the length of the soil column (Lorentz, 1987).

3.3.5 Anion exclusion

In some cases part of the liquid phase, especially near the solid end, does not participate in the transport processes. This occurs when anion exclusion takes place, or when relatively immobile liquid regions are present in the soil, for example, inside aggregates (Leij and Genuchten, 1999). Certain anions interact with the solid phase of the soil and are excluded from liquid zones adjacent to negatively charged soil particle surfaces (Shukla and Cepuder, 2000). Soil clay particles and humus surfaces exhibit negative charges that repel anions electrostatically. Anions are repelled from such surfaces and accumulate in the centre of pores. Thus, the volume of immobile water into which anionic solutes can diffuse is effectively decreased. The resultant reduction in anion concentration close to particle surfaces, which result from repulsion by electrostatic forces, is termed anion exclusion (Hall, 1993). Wild (1981) reported that anion exclusion resulted in a 10-20% reduction in pore volume available for anion transport when compared to that available for cations.

The above effect of anion exclusion suggests that anions move more rapidly than cations. For example, a study by Leij and Genuchten (1999) based on analysis of break-through curves for an anion (Cl^-), a nearly non-reactive solute (^3H_2O), and an adsorbing solute (Ca^{2+}) has shown that the Cl^- curve was strongly affected by anion exclusion, with a consequent shift of its BTC to the left, while ^3H_2O transport was subject to relatively minor adsorption or exchange. The different types of break-through curves observed for the three solutes are shown in Figure 3.3.

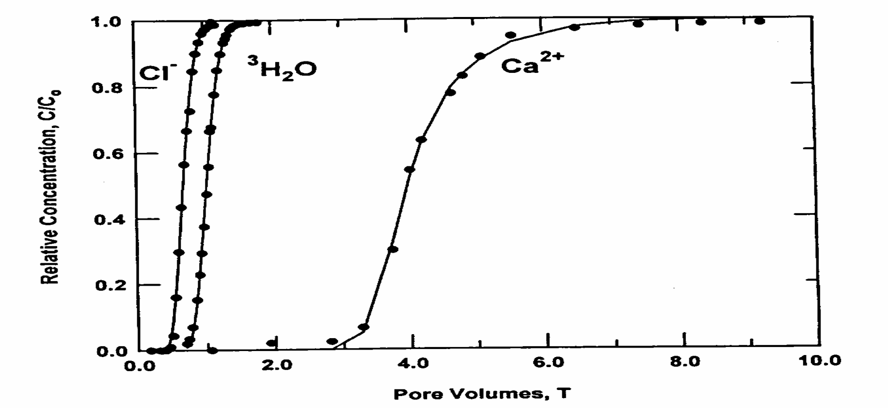


Figure 3.3 Break-through curves for Cl^-, ^3H_2O and Ca^{2+} (after Leij and Genuchten, 1999)

The main factors affecting anion exclusion are as follows (Ross, 1989; Herald, 1999):

- Anion exclusion increases with increasing anion concentration.
- Exclusion increases with increasing anion valency. More electronegative ions will be more strongly repelled by the soil particle surfaces, and to a greater distance, than less electronegative ions.
- Exclusion decreases with soil pH, since this decreases the net negative charge on soil colloids. At low pH, there are more hydrogen (H^+) ions in solution, which readily occupy the cation exchange sites, rendering the soil particle neutral. The particles will no longer be able to repel anions, hence reducing the anion exclusion effect.
- Exclusion also decreases with increasing cation saturation of the soil. This is a similar effect to increased pH, except the exchange sites are filled with cations other than H^+.
- Exclusion increases with increased density of negative charge on the particle surface. This means the particle can exert a greater repulsive force on the anions.

In general, most mechanistic solute transport models use the convection-dispersion equation to describe salt movement and leaching in the soil. However, this solute transport equation is difficult to solve numerically, largely because the mathematical properties of the transport equation vary according to the dominance of specific terms in the equation under particular situations. Moreover, this equation does not account for different management practices and soil properties. Shouse *et al.* (1997), for example, have observed large differences in water flow and salt transport between two soils with different shrink-swell characteristics. They further noticed that the salt distribution and transport in the non-cracking soil were consistent with the generally accepted principle of water and chemical transport through porous media. Conversely, this theory of water and salt transport through porous media was found to be less adequate in describing the flow of solutes through soils with large cracks that appeared as the soil dried out. This is because by-pass flow provides the primary mechanism for leaching on a heavy clay soil (Crescimanno *et al.*, 2002). Thus, the generally accepted concepts describing salt movement and leaching typically described in textbooks do not account for soils that are highly susceptible to serious cracking (Rhoades *et al.*, 1997). Some of the simplified solute transport modelling approaches are described below.

3.4 Simplified Modelling Approaches of Soil Salt Balance and Movement

Simplified approaches to assessing the soil total dissolved solute (TDS) balance have been used, ranging from simple empirical equations to conceptual functional models like the DISA hydrosalinity model. Some of these approaches are described in the following sections.

3.4.1 Empirical and simplified functional approaches

According to Aswathanarayana (2001), a steady-state value of soil salinity (*ECe*) resulting from the application of water with conductivity (*ECw*) can be estimated from knowledge of the leaching fraction (*LF*). *LF* is the fraction of applied volume of water leached below the root zone. Soil salinity in the root zone can be computed from *ECw* of applied water as:

$$ECe = X(LF) * ECw \tag{3.6}$$

where *X(LF)* is an empirically estimated parameter based on experience with irrigated, cropped soils. Some of these empirically determined *X(LF)* factors for different values of *LF* and applied water are presented in Table 3.2. These concentration factors are determined using a constant crop water use pattern along the soil profile (Ayers and Westcot, 1985).

Table 3.2 Concentration factors, *X(LF)* for predicting soil salinity, *ECe* (Ayers and Westcot, 1985)

Leaching Fraction *LF*	Irrigation Water Needed (% of total evaporation)	Concentration Factor *X(LF)*
0.05	105.3	3.2
0.10	111.1	2.1
0.15	117.6	1.6
0.20	125.0	1.3
0.25	133.3	1.2

Soil vertical heterogeneity complicates the analysis of salt transport, and a complete description of the mechanism often requires that each soil horizon be examined separately

(Schwartz *et al.*, 1999). Some researchers have adopted a modelling approach that takes into account this heterogeneity. Laudelout (1975), for example, has described a simplified salt transport and mixing model, in which the soil profile is partitioned into a number of layers. The movement of water is expressed by the fact that a given layer fills up to saturation and then empties into the layer below, returning to drained upper limit (DUL) before filling up again. If the saturation content of layer i is denoted by SP_i and its DUL by Fc_i then, applying mass conservation to each layer and supposing that perfect mixing occurs in each layer, the salt concentration of a given layer i at present time step j is expressed as:

$$C_{i,j} = [1 - (\frac{Fc_i}{Sp_i})]\, C_{i-1,j} + (\frac{Fc_i}{Sp_i}) C_{i,j-1} \qquad (3.7)$$

The drawback of this model, however, is in its inherent assumption that a given layer fills up to saturation and then drains the water above its DUL into the layer below. However, drainage of the excess water is unlikely to be an instantaneous process. Moreover, this expression does not take into account that in the case of a multi-layered soil at any time step; a given layer may receive percolated water, not only from its immediate upper layer but also from two or more overlying layers. This consideration is particularly important when longer time steps are used. The salinity level of water draining from different layers varies according to the governing processes operating on a specific layer. Although some of the simplifications of this expression are unrealistic in most cases, there is a fairly wide use of this formulation, since the retention factor defined by Fc/Sp will be close to 0.5 for most soils (Laudelout, 1975). A more rigorous functional salt balance model with water and salt movement from multiple layers is described below.

3.4.2 Soil water and TDS balance modelling in the DISA hydrosalinity model

DISA is the acronym for the Daily Irrigation and Salinity Analysis model which was developed by Ninham Shand Inc based on extensive research that had been conducted in the Breede River basin (Wolf-Piggott, 1995). Some of the underlying modelling concepts and assumptions of DISA with respect to subsurface water and TDS balance include (NSI, 1990) the following:

- The irrigated soil profile consists of a layered soil structure, allowing for a root zone, unsaturated zone and a saturated zone.
- The model takes into account the capillaric rise of water and salts in the unsaturated zone
- Movement of water between layers occurs only when the DUL is exceeded and it depends on a percolation factor.
- Groundwater movement in the saturated zone is controlled by a one dimensional Dupuit approximation.

According to Görgens *et al.* (2001), the soil profile in the model is divided into a number of layers of equal thickness. Each layer is broken down into smaller units in a horizontal plane. These units define the basic scale at which the model calculates the movement of water and salt within the root zone. In general a similar concept to that of *ACRU'*s soil water budgeting was adopted in DISA to describe water movement in the soil profile.

After calculating the soil moisture balance of each layer at the end of the day, the model determines the corresponding final salt concentration within each unit from a consideration of the salt concentration of the soil moisture at the end of previous time step, the salt concentration of inflowing and percolating (out flowing) water and soil moisture status at the present time step.

In order to ensure a realistic simulation of salt movement within the soil profile, the model divides the total volume of water entering a unit (layer) into sub-volumes, each with a different salt concentration, depending on the unit from which the water originated. Figure 3.4 is a diagrammatic representation of salt movement within the root zone. It shows that if the volume of water that enters a unit (*Qin*) is more than the initial soil moisture content of the unit immediately above, $SMCs_{(i-1)}$ (with corresponding salt concentration $Ss_{(i-1)}$), the remaining excess water from that entering the unit, after deducting the initial soil moisture content of the unit immediately above, has a salt concentration equal to that of the layer immediately above the overlying unit $Ss_{(i-2)}$. If *Qin* is more than ($SMCs_{(i-1)}$+ $SMCs_{(i-2)}$), the process continues until the total volume which constitutes *Qin* has been accounted for.

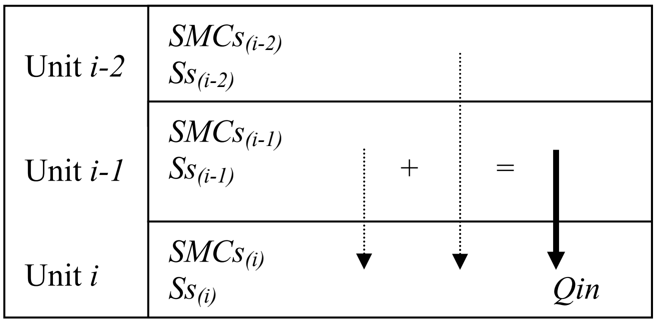


Figure 3.4 Salt movement in the soil profile (after Görgens *et al.*, 2001)

3.4.3 Salt generation

Salt generation in a soil horizon is the result of different weathering processes, mainly chemical weathering taking place in the soil profile with a subsequent release of solutes to the soil solution. Some of the chemical processes involved during weathering of rock and soil materials include hydrolysis, hydration, carbonation, dissolution and precipitation.

The level of salt generation models ranges from simple regression equations that simulate salt generation without having a clear understanding of the underlying processes to complex models that account the chemical processes taking place in the soil profile. According to Jonker (1995), various hydrosalinity models have adopted different approaches to simulate salt generation. Some of these models attempt to account for chemical processes in great detail. The LEACHM (Wagenet and Hutson, 1989) model, for example, uses a mechanistic approach, requiring detailed field information and is suited for small-scale application.

3.4.3.1 Salt generation in DISA model

According to Görgens *et al.* (2001), the DISA model does not account for dynamic salinity related soil processes such as chemical weathering processes. Although this simplification does not significantly affect the results when the model is used for single season simulations, with multiple seasons the simulated salinities in the system do, however, experience a steady decline from the second season onwards. Therefore, an attempt was made to develop a salt generation function in DISA so as to obtain a realistic representation of salinity for simulation periods of more than one season. The salt generation function is based on a simple empirical equation, which was expressed by Jonker (1995) as

$$Sgen = a(1 - e^{-bQin}) \qquad (3.8)$$

where $Sgen$ = total daily salt mass generated per soil layer (t.ha^{-1}.d^{-1})

a = calibration constant (upper limit for water percolation-related salt mass generated) (t.ha^{-1}.d^{-1})

b = constant controlling water percolation-related salt mass

if $Cin > 50$, then b=1/ln C_{in}

if $Cin \leq 50$, then b=1/ln 50

C_{in} = TDS concentration in water infiltrating the layer (mg/l)

Q_{in} = daily volume of water infiltrating the layer (l).

Development of the salt generation function in DISA is governed by various principles. Some of the principles underlying this function are given below (Jonker, 1995; Görgens *et al.*, 2001):

- The mass of salt generated in the soil profile increases asymptotically with the volume of water infiltrating the soil profile, up to a limit above which more water does not generate more salt.
- The mass of salt generated depends on the salt concentration of the water entering the soil. As shown in the preceding equation the constant, *b* depends on concentration of water infiltrating to the layer (C_{in}). The higher TDS concentration of infiltrating water, the smaller value of calibration constant (*b*) and thus the lesser salt generated will be.
- The function accommodates net salt dissolution rather than the precipitation of salts. This is based on the assumption that in an irrigation scheme where water is applied continuously, more salt is being dissolved than precipitated and it is this difference (net dissolution) that is being modelled.
- It further assumes that there exists an infinite solid salt reservoir in each layer from which salt is dissolved by the infiltrating water, instead of a finite soluble salt store.

3.4.3.2 Combined salt generation and mixing models

First order equations generally have a widespread use in describing practical chemistry related processes, as in studies of biochemical reactions and weathering processes. According to Ross

(1989), many of the processes involved during weathering of rock and soil materials are controlled by chemical kinetics. These processes include adsorption of reactants on the surface of the weathering material, chemical reactions on the surface and desorption of products from the surface. Ferguson *et al.* (1994) have proposed the application of first order rate kinetics to simulate an increase in salt concentration of the soil solution due to solute uptake by the soil water. Hence the model indirectly simulates salt generation. This solute uptake process based on first order kinetics with subsequent simple mixing of the "new" and enriched "old" water is reviewed in this section.

The salt uptake by soil solution (salt generation) model is based on first-order kinetics where the rate of increase over time in the concentration, *C*, of a solute is proportional to how far *C* falls short of its equilibrium value C_e. Introducing the rate constant (*k*) this may be expressed as:

$$\frac{\partial C}{\partial t} = k(Ce - C) \tag{3.9}$$

This equation describes an initially rapid, but progressively slower, uptake of solute so that the concentration approaches asymptotically a maximum value C_e (Figure 3.5). The rate of uptake is controlled by the rate constant *k*.

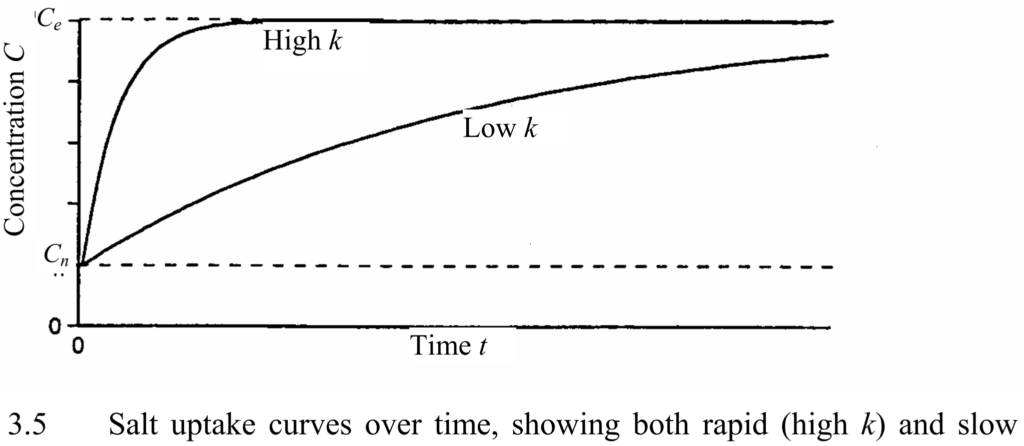


Figure 3.5 Salt uptake curves over time, showing both rapid (high *k*) and slow (low *k*) salt uptake (after Ferguson *et al.,* 1994)

The variable mixing of chemically dilute "new" (event) water (Q_n) with more enriched "old" (pre-event) water (Q_0) has been reported by different authors (e.g. Walling and Webb, 1986).

These concepts can be represented in the case of conservative mixing by $Q = Q_n + Q_0$ and the associated mixture concentration by the following equation:

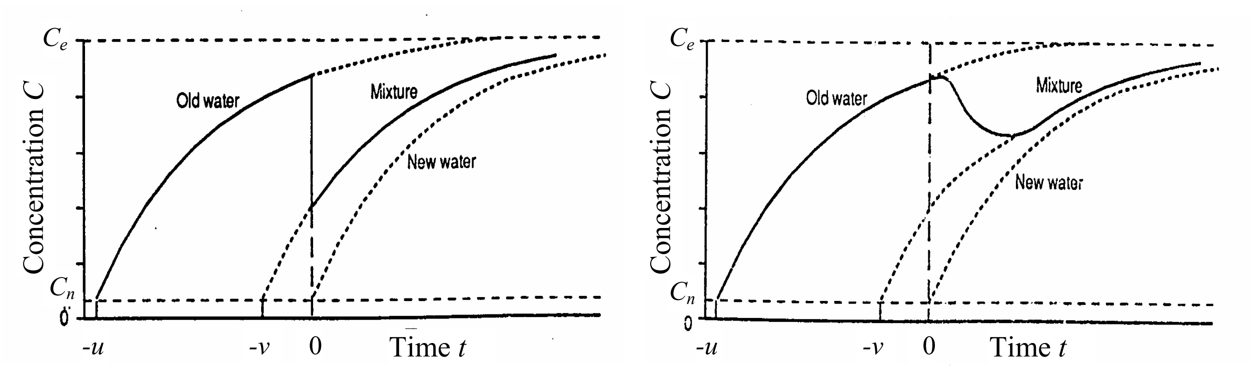
$$C = C_n R + C_o(1 - R) \tag{3.10}$$

where subscripts n and o refer to "new" and "old" water respectively and R is the volumetric ratio of "new" to "old" water (Q_n / Q).

Between rainfall or irrigation events, the water in the ground is enriched chemically. During an event this "old" water is mixed with "new" water. The mixture becomes enriched until the next event, as shown in Figure 3.6 (a). This conceptual model combines the solute mixing and uptake models, and is represented mathematically as:

$$C = C_e - (C_e - C_n)\exp(-kt)[R + \exp(-ku)(1 - R)] \tag{3.11}$$

where t and u respectively refer to age of the "new" water and that of "old" water before the occurrence of the new event. Equation (3.11) describes mixing with uptake under instantaneous events. However, mixing is unlikely to be instantaneous, first, since rainfall or irrigation are not instantaneous and secondly, as a result of the time taken for the "new" water to infiltrate and mix with the "old" soil water. Consequently, the concentration will not drop immediately to the value given by the preceding equation. Rather it will decline slowly to a minimum and then increase as shown in Figure 3.6 (b).



(a)

(b)

Figure 3.6 Sequence of enrichment of "old" water prior to an event: (a) instantaneous mixing of "new" water during an event and (b) non-instantaneous mixing (after Ferguson *et al.*, 1994)

3.5 Conclusions

From the various studies reviewed in this chapter it can be concluded that mechanistic solute transport models are more efficient in terms of describing the fundamental physical processes involved in the transport of solutes when compared to functional models. However, most mechanistic models do not take into account the impact of various management and land use practices. Moreover, because of the significant influence of field heterogeneity such as variability in soil hydraulic properties, and due to difficulties involved in obtaining the necessary soil, water and salt measurements required for mechanistic models, a simplified modelling procedure seems to be more appropriate for most management purposes.

Most of the hydrosalinity models commonly used in South Africa operate as lumped models. However, hydrosalinity studies at a catchment level usually require discretization of the catchment into a number of sub-catchments (distributed hydrosalinity modelling) in order to accurately model the impact of various land uses and water resources developments. Such distributed hydrosalinity modelling is particularly important in areas with complex land use or soils and in bigger catchments. Therefore, this calls for a conceptual-physical based hydrosalinity model that can operate both as lumped and distributed model. The following chapter will review the background and concepts of the *ACRU* agrohydrological modelling system, into which a hydrosalinity module has been developed in this project.