SOLUTE DISPERSION IN SOIL

A Thesis

Presented to

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by

KOFI BUDU LARYEA

In partial fulfilment of requirements

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ABSTRACT

SOLUTE DISPERSION IN SOIL

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An experimental study of solute transport during one-dimensional sorption of a solution of KCl into a uniformly packed horizontal soil column of Akuse clay, (a tropical clay loam from Ghana which is dominantly montmorillonitic) and Brookston clay of the Huron Catena (dominantly illitic) is reported in this thesis. A hydrodynamic equation based on the existing theories of irreversible thermodynamics is developed to incorporate the effect of anion exclusion in the usual hydrodynamic equation for one-dimensional flow of solute in soil. This equation is used to calculate the longitudinal dispersion coefficient D_s in horizontal infiltration experiments where anion exclusion effects were observed. Also, the analysis of hydrodynamic dispersion during one-dimensional horizontal flow developed by Smiles et al. (1978) is extended to include gravitational effects present during one-dimensional vertical infiltration by using the power series form of solution developed by Elrick et al. (1979). Simulation methods using computer programs written in system/360 Continuous System Modeling Program (CSMP) are used to solve the equations used in this study. The longitudinal dispersion coefficient is in all the analyses presented in this study, assumed to be independent of the Darcy flux and a function of the water content only.

In all experiments, both the soil solution content, the chloride concentration and the potassium concentration preserved similarity in

terms of distance divided by square root of time. This confirmed the assumption that the longitudinal dispersion coefficient is effectively independent of the Darcy flux for the conditions of the experiments reported in this study. These results were found to be consistent with the studies of Saffman (1959), Pfannkuch (1963) and Scotter and Raats (1970). The observed incomplete piston-like displacement of the antecedent water content suggests the presence of stagnant or 'immobile' water fractions in the soil columns considered.

The derived longitudinal dispersion coefficient for Cl^- agreed fairly well with the derived longitudinal dispersion coefficient for K^+. This is an indication that under the experimental conditions imposed, the equilibrium adsorption isotherm used to describe the adsorption term in the hydrodynamic equation for solutes which interact with soil particles, is adequate.

Simulation of water content, chloride concentration and concentration of K^+ as a function of $\lambda(=xt^{-1/2})$ using derived data $D(\lambda)$, $D_s(\lambda)$ for Cl^- and $D_s(\lambda)$ for K^+ showed very good agreement with experimental data. The simulated $c(\lambda)$ for Cl^- also showed excellent agreement with calculation of $c(\lambda)$ using a program for the analytical solution.

Water content profile and chloride concentration profile obtained for vertical infiltration experiments indicated good agreement with theoretical water content and Cl^- concentration profile simulated with CSMP. The theoretical chloride concentration profiles showed a progressively dispersed 'front' with long infiltration time periods whereas the theoretical water content profiles for various time periods showed a sharp and abrupt wetting front.

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a	radius of a cylinder in the Taylor model, L
b	half the thickness of liquid films, L
b_{ex}	thickness of the exclusion layer, L
c	concentration in solution, keq./L^3
c_{Cl^-}	concentration of chloride in solution, keq./L^3
c_{K^+}	concentration of potassium in solution, keq./L^3
c_e	local equilibrium concentration, keq./L^3
c_{ei}	equilibrium concentration at inlet end of soil column, keq./L^3
c_o	concentration at $\lambda=0$, keq./L^3
c_m	mean measured concentration, keq./L^3
C_2	reduced concentration in solution, dimensionless
D	soil water diffusivity, L^2/t
D_h	hydrodynamic dispersion coefficient, L^2/t
D_m	molecular diffusion coefficient, L^2/t
D_s	dispersion coefficient, L^2/t
g	gravitational acceleration, L/t^2
h	matric potential, L
j_i	flux of component i, M/L^2t
j^D	diffusion flux, L/t
j^v	macroscopic volume flux, L/t
keq	kilo-equivalents
kg	kilograms
K	hydraulic conductivity, L/t
l	litre
L	length

L_{ij}	phenomenological coefficient relating the flux of component i due to a force on component j
m	meter
me	milliequivalent
meq	milliequivalent
M	molar
P	pressure within the liquid phase, M/Lt^2
P_e	Péclet number
q_s	flux of salt, keq/L^2t
r	distance measured radially from the centre of the capillary tube, L
R	universal gas constant, ergs/mol. C
s,t	time, t
S	amount of solute adsorbed per mass of soil, keq./M
T	absolute temperature, T
U	velocity of the fluid at a radial distance from the axis of the tube, L/t
U_o	maximum velocity at the axis of the tube, L/t
u	pore water velocity, L/t
u^*	reduced pore water velocity, $L/t^{1/2}$
v	Darcy flux, L/t
v_i	local velocity of component i, L/t
$\bar{V}_k$	partial specific volume of the constituent k, L^3/M
x	space variable in the fixed coordinate system, L
z	depth, L
β	correction term, dimensionless

θ	volumetric water content, dimensionless
Θ	reduced volumetric water content, dimensionless
λ	horizontal distance from source divided by square root of time, $L/t^{1/2}$
$\tilde{\mu}_k$	total thermodynamic potential of component k, L^2/t^2
μ^c	concentration dependent part of $\tilde{\mu}$, L^2/t^2
ν	kinematic viscosity, L^2/t
π	osmotic pressure, M/Lt^2
ρ	bulk density, M/L^3
ρ_k	density of component k, M/L^3
σ	entropy production, M/Lt^3T
σ	reflection coefficient, dimensionless
ϕ_k	volume fraction of component k, dimensionless
ϕ_k^1	local volume fraction of component k, dimensionless
χ_k	distance divided by time for component k, L/t
ψ_k	distance divided by time to power 1.5 for component k, $L/t^{3/2}$
ω_k	distance divided by time squared for component k, L/t^2

CHAPTER 1

INTRODUCTION

The understanding and description of the simultaneous transport of solutes and water through porous media is of vital importance to science and to mankind in general. Almost all the models employed to describe the movement of solutes in porous media make use of the solute dispersion phenomenon. Consequently, understanding solute dispersion is central to the prediction of the fate of solutes during movement through porous media.

In modern agriculture, frequent applications of large quantities of water soluble materials like fertilizers and pesticides are made on the surface of the soil. Part of these materials remains in the root zone and part is carried underground by the flowing water. In order to estimate the magnitude of the hazard posed by some of these chemicals, it is important to investigate the processes that control their movement from the soil surface through the rootzone to the ground water table. Drainage, evaporation, infiltration and plant uptake studies all involve movement of chemicals through the soil. Also, the practice of leaching salts from surface layers of soil, either to lower depths or out of the soil profile, involves movement of chemicals.

In addition, there are a number of other disciplines which are involved with the transport of chemicals through porous media and hence are concerned with the phenomenon of dispersion in porous media. For example, petroleum engineers interested in secondary recovery processes and sanitary engineers need to know more about chemical and microbiological transport in soils, particularly when dealing with problems concerning waste disposal, dumps, land fills and septic tanks. Also, hydrologists need to know more about solute dispersion since they usually use tracers to study groundwater movement and aquifer parameters. Fried and Combarnous (1971) in their comprehensive review have described salt water intrusion into coastal aquifer and seepage from industrial refuse heaps and decanting tanks in which the basic information of dispersion is necessary in order to predict the movement of the various chemicals. Furthermore, as pointed out by Fried and Combarnous (1971), "... the historical development of dispersion theories offers a good background of the various modeling techniques of porous media." As a consequence, a study of dispersion is important not only because of its contribution to solving problems of practical value but also because of its importance in the design of modelling experiments.

Before proceeding further, it is necessary to qualitatively define dispersion. Dispersion refers to all the physical phenomena which govern the evolution of a transition zone when a fluid originally in a porous medium is displaced by another, both fluids being miscible. Many physical phenomena contribute to dispersion, namely, diffusion, velocity distribution within one pore geometry, velocity distribution between different pore geometries in a medium, dead end pores, flow of fluid in most pores taking place at an angle relative to mean direction of water flow and salt sieving effects (Kemper, 1960; Krupp et al., 1972).

Traditionally, investigations in movement of chemicals by dispersion through soils have been carried out mainly by analysing the concentration of the effluent, usually by fraction collection in laboratory experiments at the bottom of a column of soil in a miscible displacement apparatus (Day, 1956; Day and Forsythe, 1957; Nielsen and Biggar, 1961; Elrick and French, 1966). The behaviour of the chemical within the column was then interpreted by examining the concentration of the ion specie in the effluent by using a breakthrough curve*. In a few cases, tracer concentrations have been determined, in situ, as for example the conductivity measurements of Miller and King (1966), the "gamma emitting radioisotope" method of Shalhevet and Yaron (1967), the radiation technique used by Corey et al. (1970) and also by Kirda et al. (1974). These in situ measurements, however, have inherent problems due principally to the relative thickness of the measuring probe in comparison with the dimensions of the soil column.

Literature to date reveals that in many of the studies concerning solute movement, the tracer was assumed to be inert with respect to its environment, so that interactions with the soil matrix were often ignored. In addition, most of these studies have been limited to situations in which the soil or porous material is either completely saturated with solution or has a constant unsaturated water content, with the result that the convective motion was always assumed to be steady state. Very little work has been done which considered the behaviour of a reactive solute in a plane within the soil column. Biggar and Nielsen (1963), Kay and Elrick (1967) considered the case of adsorption during

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* A breakthrough curve is the relationship between the ratio of concentration c/c_o and the number of pore volumes V/V_o, where c is the concentration of the solute in the effluent, c_o is the concentration of the solute in the displacing fluid, V is the volume of the effluent collected and V_o is the volume of the porous medium occupied by the fluid.

movement but again these authors interpreted the behaviour of the adsorbed species by considering the concentration of the effluent.

Quite recently, Smiles *et al*. (1978) and Smiles and Philip (1978), using horizontal infiltration measurements, have shown that both the salt concentration in solution and volumetric moisture content were unique functions of $xt^{-1/2}$, where x is the horizontal distance from the absorbing surface and t is the absorption time. Elrick *et al*. (1979) used the pertubation procedure of Philip (1957) to solve the partial differential equation for salt flow during vertical infiltration of a solution of salt into a soil column.

The purpose of the present study is to investigate the dispersion phenomenon in two clay soils with a view to greater understanding of predicting the fate of solutes during flow in porous media. The research programme was designed to:

(a) extend the method of Smiles *et al*. (1978) to study the movement of a reacting solute (potassium in this case) during horizontal infiltration in soil;

(b) modify the convective-dispersion equation to include salt sieving and to use this modified equation to calculate the dispersion coefficient in a flow system where salt sieving occurs;

(c) simulate the water and salt distribution in the horizontal soil column using the calculated dispersion coefficients from the horizontal infiltration experiments and a computer program written in system 360 Continuous System Modeling Program (CSMP);

(d) simulate the water and salt distribution during vertical infiltration for a specified time by using the data from the horizontal infiltration experiments and the mathematical analysis of Philip (1957) and Elrick *et al*. (1979).

CHAPTER 2

REVIEW OF LITERATURE

Soil systems, like all porous media, are comprised of voids and solids which are not necessarily randomly distributed in size and space. Consequently, flow of fluids in the structure of soils is extremely difficult to investigate using mathematical analyses. In order to enable mathematical treatment, the true system is usually replaced by a fictitious space which is "small enough to meet practical purposes and complex enough to allow accurate description "(Fried and Combarnous, 1971). This simpler space termed a conceptual model, is generally a set of characteristics derived from experimental or theoretical considerations which are mathematically related. A conceptual model can be physical, mathematical or statistical in nature. Fried and Combarnous (1971) define physical models as those in which relationships between characteristics are derived from physical experiments while mathematical models derive their relationship between characteristics from a set of equations; for example, partial differential equations.

Many researchers, in seeking to understand and to determine dispersion, have developed various conceptual models of transport of soluble matter in soils. While some of these models include the effects of both hydrodynamic dispersion and molecular diffusion, others consider only hydrodynamic dispersion assuming the effects due to molecular diffusion to be minimal. What is more, most of these models have restrictive assumptions thus reducing their applicability to many porous media. Historically, two main developments in the study of dispersion may be delineated; namely,

(i) development of conceptual models to facilitate understanding of the dispersion process, and

(ii) laboratory and recently, field experiments aimed at utilizing one or the other of the conceptual models. The review of literature which forms the substance of this chapter will cover some of the important landmarks in the development of both the conceptual models and laboratory experimentation.

2.1 Dispersion in Capillary Tubes

Due to a similarity between a pore in a porous medium and the cylindrical space in a capillary tube, the first theoretical works on dispersion considered diffusion studies in capillary tubes. Among the early workers, Taylor (1953, 1954) formulated an expression for the description of the dispersion of salt based on observations of the dispersion of soluble matter in solvent flowing slowly through a capillary tube.

In a cylinder of radius a, depicted in figure 2.0, the distribution of velocities U(r) in a cross section is parabolic and obeys the relationship

$$U(r) = 2U_o(1 - {r^2}/{a^2}) \qquad (2.1a)$$

where U(r) is the velocity at a distance r from the axis of the tube and U_o is the maximum velocity on the axis of the cylinder. Suppose a capillary tube is filled with one fluid and a second fluid is injected at one end of the tube. Assuming the two fluids are of the same viscosity, flow is laminar and diffusion effects are of no significance, then the concentration of the displacing fluid in the effluent stream is determined by integrating the flow equation for laminar conditions. Injected fluid will not appear in the effluent stream until one-half of the tube volume is injected. For continued injection Perkins and Johnston (1963) give the instantaneous average concentration of the effluent as:

$$V_f = 1 - \left(\frac{V_t}{2V_d}\right)^2 \quad ; \quad \left(\text{when } V_d \geq \frac{V_t}{2}\right) \qquad (2.1b)$$

where V_f is the volume fraction of injected fluid in the effluent; V_t is the total volume of the tube and V_d is the volume of the fluid injected.

In actual case, molecular diffusion and hydrodynamic dispersion will cause mixing along the interface. As a consequence, the zone of mixing will be narrower than calculated from the convection effects alone because of transverse (or lateral) diffusion.

Theoretical equations derived by Taylor (1953) showed that if one fluid was displaced by another fluid under conditions where diffusion could nearly damp-out radial concentration variations, then a symmetrical longitudinal mixed zone would be established. The mixed zone would travel with the mean speed of the injected fluid and would be dispersed as if there were a constant dispersion coefficient k, which is related to molecular diffusion coefficient D_d by the relation:

$$k = \frac{a^2 U_m^2}{48 D_d} \tag{2.2}$$

where U_m equals 1/2 U_o.

In deriving equation 2.2, Taylor assumed that:

(i) the changes in concentration due to transport by convection along the tube occur in such a short time that the effect of longitudinal molecular diffusion may be neglected, and

(ii) radial differences in concentration are quickly smoothed out by molecular diffusion compared with the time necessary for appreciable effects due to convective transport to appear.

It has to be mentioned that k in equation 2.2 is a function of velocity squared.

Aris (1956) generalised Taylor's approach to irregularly shaped capillary tubes in which the molecular diffusion coefficient D_d varies with concentration, and local velocity distributions may not be parabolic. Forming moments of various order of concentration distribution, Aris developed his equations which he solved by the method of induction. He found that the moments behaved asymptotically like the moments of a normal law of probability and thus inferred that the mean concentration is dispersed according to a Gaussian distribution about a point moving at the mean velocity of flow. The variance of this distribution was used to obtain the effective diffusion coefficient K as:

$$K = D_d + \alpha[(a^2U_m^2)/D_d] \qquad (2.3)$$

In equation 2.3, α is a dimensionless number depending on the cross section of the capillary tube (for a circular cross section $\alpha = 1/48$), U_m is the mean velocity of flow, and a is the radius of the cross section.

The works of Taylor (1953, 1954) and Aris (1956) define dispersion as more than just a molecular diffusion problem.

Other geometrical models based on the capillary tube theory have been used in the past to derive flow equations. De Josselin de Jong (1958) and Saffman (1959, 1960) have both introduced random networks of capillary tubes which in some cases yield interesting qualitative results. Saffman's model which is a general case of De Josselin de Jong's, consists of a network of randomly oriented and distributed straight pores, the dimensions of which are comparable with size of pores in real porous medium and in each of which the flow is uniform. In this case, the path of each fluid particle may be considered as a random walk so that the length, direction and duration of each step are random variables. The values of the dispersion coefficient are deduced from calculation of probability distribution function of the displacement of a particle after a given time. Saffman's model was the first to account for the existence of three main domains of dispersion. namely, pure molecular diffusion, molecular diffusion and hydrodynamic dispersion of equal importance, and hydrodynamic dispersion and molecular diffusion interfering with the latter being the smaller of the two. In addition to these, Saffman's work indicates the difference in importance between lateral and longitudinal dispersion. He predicts in his work that for Péclet numbers (fluid velocity x characteristic pore size/molecular diffusion coefficient of solute in bulk solution) less than 1, the dispersivities are essentially equal to the coefficient of molecular diffusion of the solute through the medium. In other words, the effects of convection on mixing at the interface are essentially negligible. As pointed out by Peck (1971), convection may still be dominant in solute transport at Péclet numbers less than 1 because for a solute with molecular diffusivity of 10^{-9} m^2s^{-1} in a medium with characteristic pore diameter of 10^{-5} m (a very fine sand or silt), the Péclet number is less than 1 and mixing at the interface is essentially by molecular diffusion for fluid velocities less than about 10^{-4} m s^{-1}. In about 10^4 s, convective transport would move solutes a distance of about 1 m and in the same period molecular diffusion may transport the solute a distance of about 10^{-3} m.

Bear et al. (1968) and Bachmat (1969) have improved the random capillary models of De Josselin de Jong and Saffman by averaging microscopic quantities (microscopic scale is the scale of the pore) in a representative element of volume REV at a point to build a continuum at the macroscopic level (the scale of dispersion phenomenon and Darcy's Law). Their model fits experimental results closer than Saffman's model and provides a general equation for nonhomogeneous media and nonhomogeneous fluids.

All the capillary models, however, experience the same difficulties as does the Kozeny-Carman's development of a formula for calculating the hydraulic conductivity of a soil in that precise theory for simple geometry is forced to fit the complex internal architecture of a porous medium.

2.2 The Classical Statistical Models

Einstein's (1937) theory of random walk has been extended by Giddings (1959) who indicated that the spread of a solute as a result of continuous change in flow velocity of a volume element from an initially horizontal zone, obeyed the laws of statistics and could be characterised by a parameter which he called an "eddy diffusion coefficient" (now referred to as hydrodynamic dispersion coefficient). Following Giddings' work and under the assumption that

(i) the porous medium under consideration is homogeneous and isotropic,

(ii) events occurring in one elemental time step are independent of events occurring in any other time step, and

(iii) the movement of a solute obeys the laws of laminar flow,

Scheidegger (1974) presents two types of models, namely, a random walk model and a random media model. In the former, randomness is directly ascribed to the fluid particles while in the latter flow occurs along random channels.

The random walk model as proposed by Scheidegger is based on an analogy with Brownian motion. A particle of fluid is first considered to be very small such that it cannot be separated into separate channels during passage in a porous medium. Then for a fixed time T, one asks for the probability P(x,T) of finding a particle at the spot x at time T. The total time is split into small time steps t during which the progress

Figure 2.0: Capillary tube conceptual model.

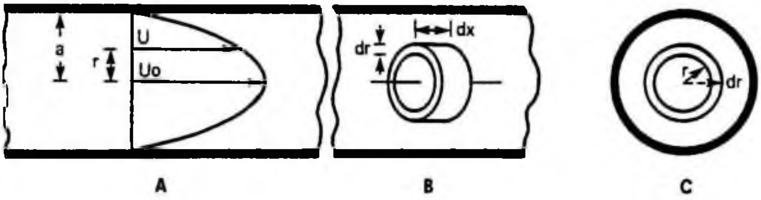

Figure 2.0

of the particle is considered a random variable. The sum of these elemental progresses yields the position of the particle at time t. Scheidegger (1974) used the central limit theorem which established conditions under which sums of independent random variables are asymptotically normally distributed to show that function P(x,T) is Gaussian. Hence it is a solution of a diffusion-type equation given for a co-ordinate system (x',T') moving with mean pore velocity of flow as

$$\frac{\partial P(x',T')}{\partial T'} = \frac{K\partial^2 P(x',T')}{\partial x'^2} \qquad (2.4)$$

The change of variables x = x'+UT' and t = T' was used to transform equation 2.4 to co-ordinates (x,t), thus obtaining

$$\frac{\partial P}{\partial t} = K\frac{\partial^2 P}{\partial x^2} - U\frac{\partial P}{\partial x}$$ which was shown to yield

$$\frac{\partial c}{\partial t} = K\frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} \; . \qquad (2.5)$$

According to the law of large numbers, the concentration in a displacing fluid in a miscible displacement is equal to the probability of finding a particle of displacing fluid at that point. K in equations 2.4 and 2.5 is a scalar called the dispersion coefficient. From experimental observations that when the concentration gradient is perpendicular to the mean flow (lateral dispersion) the dispersion coefficient is different from the dispersion coefficient observed when the concentration gradient is parallel to the mean flow (longitudinal dispersion), Scheidegger (1974) then generalised equation 2.5 to show that K is a tensor and not a scalar.

2.3 Solute Transport in Inert Porous Media

Porous media such as soils are not well represented as collections of capillary tubes since the flow paths are not canalized but are extensively cross linked. Thus in each pore in a soil several flow paths nearly coalesce and then diverge. Most of the dispersion in soils, therefore, comes from the meandering of the streamtubes through the complex structure of the medium and not from only the existence in each pore of a velocity profile as in a tube. Laboratory experiments aimed at studying dispersion in soils have been carried out in the past. A common technique of most of the experimental work is to compare theoretical curves obtained from one of the existing models or a new model with experimental breakthrough curves. If the two curves match, it is presumed that the assumptions made for the derivation of the model also hold for the experimental situation.

Most experiments are conducted with certain restrictive conditions, the usual conditions being that:

(i) the dispersion coefficient which is a tensor is reduced to its principal coefficients; i.e., the lateral dispersion coefficient and the longitudinal dispersion coefficient with boundary conditions chosen such that one of these coefficients can be neglected.

(ii) the flow is made uniform and fingering* prevented, and

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* Fingering is a distortion of the boundary between displacing and displaced fluids frequently caused by differences in density and viscosity of the fluids.

(iii) generally the initial concentration profiles are step functions.

An early experimental work which demonstrated the essence of the process of dispersion without mathematical treatment was reported by Griffiths (1911) who observed that a tracer injected into a stream of water spreads out in a symmetrical manner about a plane in the cross-section which moves with the mean speed of flow. As pointed out by Taylor (1953), (reviewed earlier in section 2.1) Griffith's observation is rather startling for two reasons. First is that since water moves at twice the mean speed near the centre of the pipe and the patch of colour at the mean speed, the clear water in the middle must approach the colour patch, absorb colour as it passes into it and then lose colour as it passes out,finally leaving the patch as perfectly clear water. The second remarkable feature is that the colour patch spreads out symmetrically from a point which moves with the mean speed of the fluid in spite of the fact that the distribution of velocity over the section, which gives rise to this dispersion, is highly unsymmetrical.

Burd and Martin (1923) observed that when distilled water is used to displace a solution from a packed column of saturated soil, the displaced solution had an almost constant composition until a substantial fraction of this solution had been displaced, then the concentration decreased gradually instead of decreasing abruptly to zero as one might expect from the sharp interface that was initially established between the original soil solution and the displacing water phase. This manifestation of dispersion was referred to as hydrodynamic dispersion by Day (1956) who demonstrated that layers of salt water displaced through a water saturated column of sand by fresh water, were distributed in accordance with the statistical theory developed by Scheidegger (1954).

One of the most well known introductions of miscible displacement technique to the field of Soil Science was made by Nielsen and Biggar in the series of papers, Nielsen and Biggar (1961, 1962, 1963) and Biggar and Nielsen (1962, 1963). Nielsen and Biggar (1962) indicated that any experimentally measured breakthrough curve in a porous medium may have the characteristic of one or a combination of the five breakthrough curves shown in Figure 2.1. If there is no interaction between the solvent, solute and the porous medium, the following relationship should hold for Figure 2.1a, 2.1b, and 2.1c, irrespective of the shape of the breakthrough curve.

$$\frac{Q}{V_o} \int_o^{\infty} \left(1 - \frac{c_e}{c_i}\right) dt = 1 \qquad (2.6)$$

where Q is the mean flow rate in $m^3 s^{-1}$

t is time in s

V_o is the volume of the porous material occupied by the fluid in m^3

c_e is the concentration of the solute found in the effluent in keq. m^{-3}

c_i is the concentration of the solute in the displacing fluid in keq. m^{-3}.

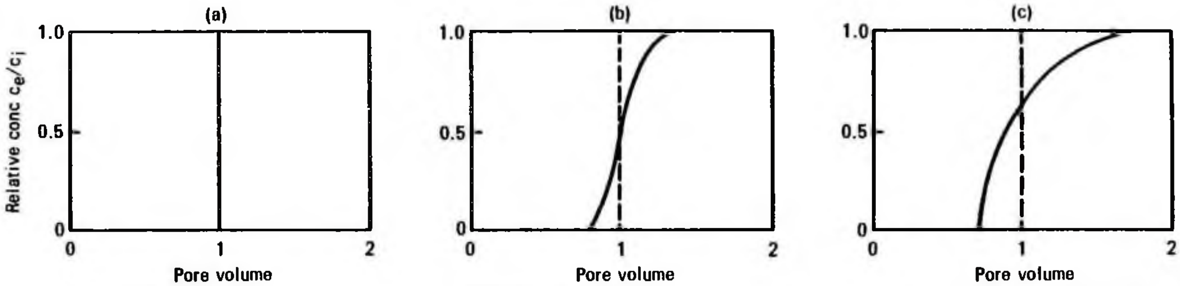
The area under the breakthrough curve up to one pore volume is, under these conditions, equal to the area above the curve beyond one pore volume. Mathematically, this requirement is expressed as

$$\frac{Q}{V_o}\int_0^{V_o/Q}\left(\frac{c_e}{c_i}\right)dt = \frac{Q}{V_o}\int_{V_o/Q}^{\infty}\left(1-\frac{c_e}{c_i}\right)dt \qquad (2.7)$$

When there is interaction between the solute and soil solids such as adsorption process, the breakthrough curve would be translated to the right of one pore volume as in Figure 2.1d. Processes within the soil which result in an increase of solute concentration or incomplete mixing throughout the soil solution would, as shown in Figure 2.1e, give a breakthrough curve translated to the left of one pore volume. Consequently, processes such as dissolution of slightly soluble salts present in porous media, incomplete mixing due to dead end pores would all translate the breakthrough curve to the left of one pore volume. Using Aiken clay and Oakley sand, Nielsen and Biggar (1961, 1962, 1963) concluded that physical differences among soils contribute to the shape and position of breakthrough curves.

It should be pointed out that the type of breakthrough curve depicted for the effects of anion exclusion and for processes within the soil which result in increase of solute concentration due to dissolution of salts present in the soil (Fig. 2.1e) by Nielsen and Biggar (1962) is inaccurate. When salt sieving occurs, one expects, as pointed out by Nielsen and Biggar (1962) a breakthrough curve translated to the left of one pore volume. The relative concentration c_e/c_i after one pore volume, however, would be smaller than 1.0 (see Figure 2.1f). In the

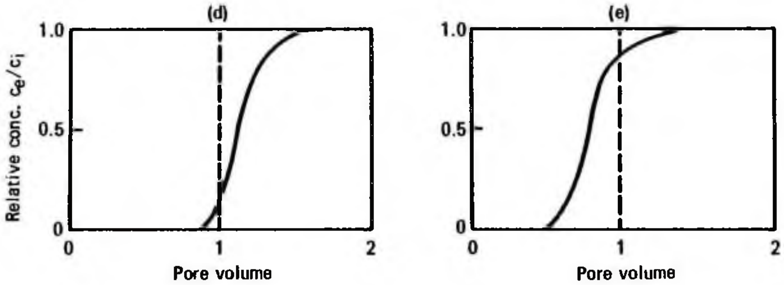
Figure 2.1: Types of breakthrough curves for miscible displacement (a to e were adapted from Nielsen and Biggar, 1962).



Piston flow

Longitudinal dispersion

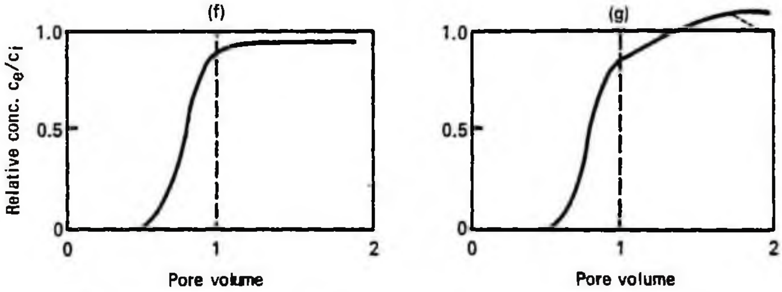
Extremely wide range in velocity distribution



Chemical reaction,precipitation or exchange

Exclusion of solute or velocity distribution with velocities near zero

Figure 2.1



Expected curve for salt exclusion

Expected curve for processes which increase solute concentration

Figure 2.1

case where processes within the soil result in increase of solute concentration, one expects relative concentration greater than 1.0 after one pore volume (Figure 2.1g). If there is a constant source which causes the increase of the solute (i.e. greater quantities of soluble salts present), then c/c_e in Figure 2.1g will flatten above 1.0. On the other hand, if the source is limited, c/c_e will, after increasing for some period beyond 1.0, creep back to 1.0.

Other workers, for example Elrick and French (1966), Elrick _et al_. (1966), Corey (1966), Corey _et al_. (1967), have also extensively employed the miscible displacement technique to study movement of mostly non-interacting solutes such as chloride or nitrate in porous media.

2.4 Transport with Exchange or Adsorption in Porous Medium

The dispersion phenomenon may be complicated by the occurrence of clay in the porous medium because surface reactions such as adsorption may occur.

Adsorption is a process in which matter is extracted from one phase and concentrated at the surface of a second and as such it is termed a surface phenomenon (Weber, 1972). For most systems three principal types of adsorption may be identified: physical adsorption resulting from van der Waals attraction; chemical adsorption and exchange adsorption resulting from electrostatic attractions to charged surface sites on the solid. The factors affecting adsorption include the specific surface area of the solid, the concentration and the nature of competing ions, pH and the nature of the adsorbent. Generally, adsorption and/or exchange reactions are of prime importance in most agricultural soils where cations usually interact with the negatively charged clay surfaces or replace other cations already on the clay surface through cation exchange reaction.

The diffusion-like description of dispersion in porous media has in the past been modified to include the effects of simple reversible exchange or adsorption of solute on the medium so that the equation of continuity for the exchange of solute between a mobile phase and a soil column is usually taken as

$$\frac{\partial c}{\partial t} + U_m \frac{\partial c}{\partial x} = D_s \frac{\partial^2 c}{\partial x^2} - \frac{1}{\gamma} \frac{\partial S}{\partial t} \qquad (2.8)$$

where U_m is the mean pore velocity

γ is the void fraction and

S is the amount of solute adsorbed per unit volume of the packed soil.

At a point in a porous medium system, adsorption results in the removal of solutes from solution and their resulting concentration at the surface of the solid, to such time as the concentration of the solute remaining in solution is in dynamic equilibrium with that at the surface. The term $(\frac{1}{\gamma} \frac{\partial S}{\partial t})$ in equation 2.8 represents the exchange of solute between the phases and is evaluated either by using a finite rate of adsorption equation or by introducing the concept of instantaneous equilibrium when values of S at each position, x, would be given by the adsorption isotherm $S = f(c)$.

Lapidus and Amundson (1952) have considered both cases of equilibrium adsorption and kinetic reaction for a semi-infinite column ($0 \leq X < \infty$) where a continuous solute flux at the surface was treated as a boundary condition (c = constant at $X = 0$). The rate equations used were

$$S = k_1 c + k_2 \tag{2.9}$$

in which k_1 and k_2 are constants, and

$$\frac{\partial S}{\partial t} = k_3 c - k_4 \tag{2.10}$$

where k_3 and k_4 are the rate constants. Equation 2.9 indicates the condition of local equilibrium between the fluid and solid phase at all points in the porous medium and also linearity of the adsorption isotherm. Equation 2.10, however, is a non-equilibrium first order kinetic relationship and implies that the rate of adsorption is finite.

Following Lapidus and Amundson (1952), Houghton (1963) has treated mathematically the dispersion phenomenon assuming an equilibrium between the adsorbed and solution phases and a non-linear isotherm of the polynomial form

$$S = f(c) = K_0 + K_1 c + K_2 c^2 \tag{2.11}$$

As indicated by Houghton, this form of isotherm has the advantage that it is concave to the S-axis for positive K_2, concave to c-axis for negative K_2 and linear for K_2 equals zero. K_0 has been introduced so that equation 2.11 might be used to approximate highly curved isotherms without the use of higher order terms such as K_3c^3, K_4c^4 ...

Adopting the rate equations and mathematical solution of Lapidus and Amundson (1952), Banks and Ali (1964) presented experimental information in which the rate constants k_3 and k_4 were calculated, but failed to check for agreement between the theoretical solution and the experimental data on grounds that the theoretical solution is complex. Hashimoto et al. (1964) have also obtained a solution similar to the mathematical solution of Lapidus and Amundson (1952). This solution, which includes the longitudinal mixing process as well as equilibrium and linear adsorption during one dimensional flow, was later used by Kay and Elrick (1967) to show that at low flow rates the movement of lindane, a pesticide, in their porous material was reasonably well described by their chromatographic model. However, at high pore water velocities, Kay and Elrick (1967) and also Davidson and Chang (1972) have shown that there is considerable deviation between their mathematical models and experimental data. These two studies suggested that for high pore water velocities the use of a kinetic rate equation to describe the adsorption process may be necessary. Nonetheless, examining various adsorption models usually employed for the description of the adsorption process, Van Genuchten et al. (1974) found kinetic adsorption-desorption models to be inadequate when predicting the mobility of pesticides for high average pore water velocities. They indicate, however, that these kinetic models agreed with the equilibrium adsorption model when used to describe pesticide effluent concentration distribution at low pore water velocities.

In the past, other types of isotherms, for example, the Freundlich model and Langmuir model and also first order kinetic reactions, have been used with differing degrees of success (Lindstrom and Boersma, 1970; Swanson and Dutt, 1973; Selim and Mansell, 1976; Selim _et_ _al_., 1977).

In many practical situations, other chromatographic models have been applied (Bower _et_ _al_., 1957; Gardner and Brooks, 1957; Biggar and Nielsen, 1967). In some of these applications these models have been quite successful but other investigators have attributed discrepancies between theory and experimental data to changes of the cation exchange capacity with pH (Thomas and Coleman, 1959) and the neglect of dispersion due to convection and diffusion (Biggar and Nielsen, 1963).

It appears that the theory of the transport of a solute subject to adsorption or exchange has not been adequately tested in transient flow systems. The conclusion may, however, be drawn from examination of the partial differential equations describing the transport of solutes which interact with the soil matrix, that adsorbed and exchanged materials are transported less rapidly than those which are not.

CHAPTER 3

THEORY

3.1 Convective-dispersive equation for horizontal infiltration of water and salt

The basic assumption usually made when considering the problem of simultaneous transfer of solute and water is that the transport of the soluble matter is governed principally by molecular diffusion (thermal motion within the soil solution) and convection (viscous movement of the solution). Macroscopically, diffusion of solutes in a uniform body of water may be described by Fick's first law which states that the rate of transfer of a diffusing substance through a unit area of section is proportional to the concentration gradient measured normal to the surface through which diffusion is taking place. In differential form this law is

$$J_s = -D_d \left(\frac{\partial c}{\partial x}\right) \qquad (3.1)$$

where J_s	is the flux of solute	keq. $m^{-2} s^{-1}$
D_d	is the Diffusion Coefficient of the solute in water	$m^2 s^{-1}$
c	is the concentration of the solute in solution	keq. m^{-3}
x	is the horizontal coordinate	m.

Equation 3.1 is applicable under conditions of no liquid flow.

In soils the diffusion coefficient D_d is less than the equivalent coefficient in a free water system. Also, for practical purposes, the diffusion coefficient in a clay-water system may be considered independent of the salt concentration and dependent only on the water content (Kemper and van Schaik, 1966).

Generally, it is assumed that the macroscopic transport by convection must take into account the average flux of water as well as the mechanical or hydrodynamic dispersion. Experimental and theoretical works of Perkins and Johnston (1963) and Passioura (1971) have shown that the magnitude of the hydrodynamic dispersion coefficient D_h in a given porous medium depends on the average flow velocity and that under steady and saturated conditions D_h may often be taken to be proportional to the first power of the average flow velocity, V_s (Bear, 1961; Perkins and Johnston, 1963). This is stated in the form

$$D_h(V_s) = k|V_s| \tag{3.2}$$

where k in centimeters is an experimental constant depending on the characteristics of the porous material (especially the pore size distribution) and V_s is in centimeters per second. When the Darcy flux, v, is used, equation 3.2 is of the form

$$D_h(v) = \frac{k|v|}{\theta}$$

where θ is the volumetric moisture content.

The joint effect of diffusion and convection is combined to formulate the mathematical expression for the flux in one dimensional flow of solute as:

$$J_s = vc - \theta[D_h(v) + D_d(\theta)]\frac{\partial c}{\partial x} \qquad (3.3a)$$

$$J_s = vc - \theta D_s(v,\theta)\frac{\partial c}{\partial x} \qquad (3.3b)$$

where D_s is the combined diffusion-hydrodynamic dispersion coefficient (referred to in the rest of this thesis as the dispersion coefficient).

The nature and values of D_s have been the subject of many discussions and experiments. In equation 3.3b a tacit assumption has been made that a single constant can be used to describe both the diffusive and dispersive effects. Examination of the extreme cases, when either effect may be neglected, clarifies this. Thus, when v equals zero, $D_h(v) = 0$, and so D_s equals D_d (Bear, 1961; Perkins and Johnston, 1963). At high Darcy fluxes, the effect of molecular diffusion is normally neglected and D_s then equals D_h. The structure of D_s for intermediate situations, for example where D_d is approximately equal to D_h, is not very clear. However, for $D_d >> D_h$, additivity has been claimed on theoretical grounds (Beran, 1957). This assumption is often extended to a wide range of D_d to D_h ratio: $D_n/D_d < 50$ (Perkins and Johnston, 1963). In this study, apart from using a single term to describe the phenomenon of hydrodynamic dispersion and molecular diffusion and their possible interaction, an assumption is also made that D_s is θ-dependent but effectively independent of the Darcy flux (Smiles _et_ _al_., 1978; Smiles and Philip, 1978; Elrick _et_ _al_., 1979).

For non-steady state or transient conditions the equation describing time and space relationships of the flux of solute is derived through the use of equation 3.3b and the continuity equation

$$\frac{\partial M}{\partial t} = - \frac{\partial J_s}{\partial x} \qquad (3.4)$$

where M (keq/m^3) is the total quantity of solute in the bulk volume of soil. For a non-interacting solute M may be expressed as

$$M = \theta c \qquad (3.5)$$

For solutes that interact with the soil particle surfaces, however, M may be expressed as

$$M = \theta c + \rho S \qquad (3.6)$$

where ρ (kg m^{-3}) is the bulk density of the soil and S is the amount of solute associated with the solid phase in units of quantity of solute per mass of soil (i.e. keq/ per kilogram of soil).

Consequently, the continuity equations for non-interacting and interacting solutes become,respectively

$$\frac{\partial(\theta c)}{\partial t} = - \frac{\partial J_s}{\partial x} \qquad (3.7a)$$

$$\frac{\partial(\theta c + \rho S)}{\partial t} = - \frac{\partial J_s}{\partial x} \qquad (3.7b)$$

which when substituted into equation 3.3b with the assumption of the dependence of D_s only on θ yields for one dimensional horizontal flow:

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] - \frac{\partial(vc)}{\partial x} \qquad (3.8a)$$

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(\rho S)}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] - \frac{\partial(vc)}{\partial x} \qquad (3.8b)$$

The one-dimensional flow of water may be described by the Darcy equation of the form

$$v = -D(\theta)\frac{\partial\theta}{\partial x} \qquad (3.9)$$

where D is the soil moisture diffusivity ($m^2\ s^{-1}$) and is equal to $K\frac{\partial\psi}{\partial\theta}$, K is the hydraulic conductivity (ms^{-1}) and ψ is the matric potential (m).

In equation 3.9, the assumption has been made that there is a unique relationship between θ and ψ in the moisture characteristic curve which is not true because of hysteresis. However, if we consider only the sorption or only the desorption curve, then Darcy's equation in this form may be used. Substitution of the continuity equation for water flow

$$\frac{\partial\theta}{\partial t} = -\frac{\partial v}{\partial x} \qquad (3.10)$$

into equation 3.9 yields

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[D(\theta)\frac{\partial\theta}{\partial x}\right] \qquad (3.11a)$$

which can be transformed into the following ordinary differential equation:

$$\frac{d}{d\lambda}\left[D(\theta)\frac{d\theta}{d\lambda}\right] + \frac{\lambda}{2}\frac{d\theta}{d\lambda} = 0 , \qquad (3.11b)$$

where $\lambda = xt^{-1/2}$.

The solution of equation 3.11b for $D(\theta)$ subject to following initial and boundary conditions

$$\left.\begin{aligned} \theta(x,t) &= \theta_n \text{ for } x > 0,\ t = 0,\ \lambda \to \infty \\ \theta(x,t) &= \theta_s \text{ for } x = 0,\ t > 0,\ \lambda = 0 \end{aligned}\right\} \qquad (3.12)$$

has been given by Bruce and Klute (1956) as

$$D(\theta) = -\frac{1}{2}\frac{d\lambda}{d\theta}\int_{\theta_n}^{\theta} \lambda d\theta \qquad (3.13)$$

3.2 Solution of Equations 3.8a and 3.8b for D_s

It is observed that any analytical or numerical solution of equations 3.8a and 3.8b and subsequent prediction of the concentration distribution with time from these equations will require information on the magnitude and the dependence of the dispersion coefficient on θ, v and c. One of our objectives, as indicated earlier, is to solve equations

3.8a and 3.8b for D_s, design experiments to measure D_s indirectly, and use these D_s values to simulate the concentration distribution.

Equations 3.8a and 3.8b may be expanded as

$$c\frac{\partial\theta}{\partial t} + \theta\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] - v\frac{\partial c}{\partial x} - c\frac{\partial v}{\partial x} \qquad (3.14a)$$

$$c\frac{\partial\theta}{\partial t} + \theta\frac{\partial c}{\partial t} + \rho\frac{\partial S}{\partial t} + S\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] \quad v\frac{\partial c}{\partial x} - c\frac{\partial v}{\partial x} \qquad (3.14b)$$

Substitution of the continuity equation 3.10 into equations 3.14a and 3.14b and use of a further assumption that in equation 3.14b the bulk density ρ is constant during horizontal infiltration (that is, there is no swelling), gives

$$\theta\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] - v\frac{\partial c}{\partial x} \qquad (3.15a)$$

$$\theta\frac{\partial c}{\partial t} + \rho\frac{\partial S}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial x}\right] - v\frac{\partial c}{\partial x} \qquad (3.15b)$$

The initial and boundary conditions of interest for equations 3.15a and 3.15b are:

$$\theta(x,t) = \theta_n\ , \quad c(x,t) = c_n \quad \text{for } x \geq 0,\ t = 0 \qquad (3.16a)$$

$$\theta(x,t) = \theta_s\ , \quad c(x,t) = c_o \quad \text{for } x = 0,\ t > 0 \qquad (3.16b)$$

Condition 3.16a indicates that initially the soil column has for all values of $x > 0$, a constant moisture content θ_n and a constant concentration of salt, c_n. Condition 3.16b implies that a solution would be applied at the input end $x = 0$ at time $t = 0$ and for all times $t > 0$ and that the solution would be applied in such a way as to maintain the soil at the input end of the column at a constant moisture content θ_s and a constant salt concentration c_o.

Smiles *et al.* (1978) have shown that both the water and salt concentration profile preserve similarity during horizontal infiltration in terms of distance divided by the square root of time. Accordingly, the substitution $\lambda = xt^{-1/2}$ was shown to remove both x and t from equation 3.15a as follows:

$$\theta \frac{\partial c}{\partial \lambda}\frac{\partial \lambda}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial \lambda}\frac{\partial \lambda}{\partial x}\right] - v\frac{\partial c}{\partial \lambda}\frac{\partial \lambda}{\partial x}$$

$$-\frac{\theta\lambda t^{-1}}{2}\frac{\partial c}{\partial \lambda} = t^{-1/2}\frac{\partial}{\partial \lambda}\frac{\partial \lambda}{\partial x}\left[\theta D_s(\theta)\frac{\partial c}{\partial \lambda}\right] - vt^{-1/2}\frac{\partial c}{\partial \lambda} \qquad (3.17)$$

Substitution of equation 3.9 into equation 3.17 for v gives

$$-\frac{\theta\lambda}{2}t^{-1}\frac{\partial c}{\partial \lambda} = t^{-1}\frac{\partial}{\partial \lambda}\left[\theta D_s(\theta)\frac{\partial c}{\partial \lambda}\right] + D(\theta)\frac{\partial \theta}{\partial \lambda}\frac{\partial \lambda}{\partial x}\frac{\partial c}{\partial \lambda}\frac{\partial \lambda}{\partial x}$$

$$-\frac{\theta\lambda}{2}t^{-1}\frac{\partial c}{\partial \lambda} = t^{-1}\frac{\partial}{\partial \lambda}\left[\theta D_s(\theta)\frac{\partial c}{\partial \lambda}\right] + t^{-1}D(\theta)\frac{\partial \theta}{\partial \lambda}\frac{\partial c}{\partial \lambda}$$

$$\frac{d}{d\lambda}\left[\theta D_s(\theta)\frac{dc}{d\lambda}\right] + \left(\frac{\theta\lambda}{2} + D(\theta)\frac{d\theta}{d\lambda}\right)\frac{dc}{d\lambda} = 0 \qquad (3.18a)$$

which may be written as

$$\frac{d}{d\lambda}\left[\theta D_s(\theta)\frac{dc}{d\lambda}\right] + \frac{g(\theta)}{2}\frac{dc}{d\lambda} = 0 \qquad (3.18b)$$

where

$$g(\theta) = \theta\lambda + 2D(\theta)\frac{d\theta}{d\lambda} = \theta\lambda - \int_{\theta_n}^{\theta} \lambda d\theta \qquad (3.18c)$$

The extreme right hand term in equation 3.18c can be obtained by substituting equation 3.13 into 3.18c for D(θ). Transformation of equation 3.15b in a similar way yields the ordinary differential equation of the form

$$\frac{d}{d\lambda}[\theta D_s(\theta)\frac{dc}{d\lambda}] + \frac{g(\theta)}{2}\frac{dc}{d\lambda} + \frac{\rho\lambda}{2}\frac{dS}{d\lambda} = 0 \qquad (3.19)$$

In view of the transformation $\lambda = xt^{-1/2}$, conditions 3.16a and 3.16b may be written as

$$\theta = \theta_n , c = c_n \text{ for } \lambda \to \infty \qquad (3.20a)$$

$$\theta = \theta_s , c = c_o \text{ for } \lambda = 0 \qquad (3.20b)$$

This implies also that for $\theta = \theta_n$ and $c = c_n$, $\frac{d\theta}{d\lambda} = 0$ and $\frac{dc}{d\lambda} = 0$.

Equation 3.18b is linear in c and may be solved in the explicit form subject to 3.20a and 3.20b to obtain (Smiles et al., 1978)

$$\frac{c - c_o}{c_n - c_o} = \frac{M(\lambda)}{M(\infty)} \qquad (3.21a)$$

with

$$M(\lambda) = \int_o^\lambda \{(\theta D_s)^{-1}(\lambda) \exp[-1/2 \int_o^\lambda g(\lambda)(\theta D_s)^{-1}(\lambda)\, d\lambda]\}\, d\lambda \qquad (3.21)$$

However, we may solve equation 3.18b for $D_s(\theta)$ as follows:

If $y = \theta D_s(\theta) \frac{dc}{d\lambda}$, then

$$\frac{dy}{d\lambda} = -\frac{g(\theta)}{2}\frac{dc}{d\lambda}$$ which upon integration yields

$$y \Big|_{\lambda\to\infty}^{\lambda} = -\frac{1}{2}\int_{c_n}^{c} g(\theta)\, dc$$

Since for λ → ∞, $dc/d\lambda = 0$ we get

$$D_s(\theta) = -\frac{1}{2}\frac{1}{\theta}\frac{d\lambda}{dc}\int_{c_n}^{c} g(\theta)\, dc \qquad (3.22)$$

$D_s(\theta)$ may be calculated either from equation 3.22 using a numerical technique or, as was done in this study, from equation 3.18b directly using C.S.M.P.

In the case of reactive solutes (equation 3.19), we require a relationship between the quantity of solute adsorbed per gram of soil S and concentration of solute in solution c. A number of models of adsorption and exchange have been proposed, some representing equilibrium between c and S and other representing time-dependent adsorption processes

(Boast, 1973). In this study, the model used assumes an equilibrium between c and S. $D_s(\theta)$ was calculated from equation 3.19 using C.S.M.P. by programming the computer to fit c and S values provided, with a non-linear function. This aspect of the thesis is considered in detail in Chapter 4. However, another approach was used and a non-linear polynomial similar to that of Houghton (1963) but in logarithmic scale was fitted to the adsorption isotherm and upon substitution into equation 3.19, the resulting equation solved for D_s as follows:

The non-linear polynomial in logarithmic scale was of the form

$$\log S = -k_1 \log^2 c + k_2 \log c - k_3 \qquad (3.23)$$

where k_1, k_2 and k_3 are constants. From equation 3.23

$$S = 10^{[-k_1 \log^2 c + k_2 \log c - k_3]}$$

$$= 10^{[-k_4 \ln^2 c + k_5 \ln c - k_3]} \qquad (3.24)$$

In equation 3.24, $k_4 = k_1/5.304$ and $k_5 = k_2/2.303$

$$\frac{dS}{dc} = [\ln 10(\frac{-2k_4 \ln c + k_5}{c})]\ [10^{(-k_4 \ln^2 c + k_5 \ln c - k_3)}]$$

$$\frac{dS}{dt} = \frac{2.303}{c}(k_5 - 2k_4 \ln c)(10^{[-k_4 \ln^2 c + k_5 \ln c - k_3]})\frac{dc}{dt} \qquad (3.25)$$

Substituting equation 3.25 into equation 3.15b and transformation with $\lambda = xt^{-1/2}$ yields

$$\frac{d}{d\lambda}\left[\theta D_s(\theta)\,\frac{dc}{d\lambda}\right] = -\frac{1}{2}\left\{\theta\lambda + \frac{2.303\rho\lambda}{c}\,(k_5-2k_4\ln c)\,(10^{[-k_4\ln^2 c+k_5\ln c-k_3]})\right\}\frac{dc}{d\lambda}$$

$$- D(\theta)\,\frac{d\theta}{d\lambda}\,\frac{dc}{d\lambda} \qquad (3.26)$$

Substitution of $y = \theta D_s\frac{dc}{d\lambda}$ into equation 3.26 and integrating gives

$$y\,\Big|_{\lambda\to\infty}^{\lambda} = -\frac{1}{2}\int_{c_n}^{c}\left\{\theta\lambda + \frac{2.303\rho\lambda}{c}(k_5-2k_4\ln c)(10^{[-k_4\ln^2 c+k_5\ln c-k_3]}) - \int_{\theta_n}^{\theta}\lambda\,d\theta\right\}dc$$

which because at λ → ∞, $\frac{dc}{d\lambda} = 0$ we obtain

$$D_s(\theta) = -\frac{1}{2}\,\frac{1}{\theta}\,\frac{d\lambda}{dc}\int_{c_n}^{c}\left\{\theta\lambda + \frac{2.303\rho\lambda}{c}\,(k_5-2k_4\ln c)\,(10^{[-k_4\ln^2 c+k_5\ln c-k_3]}) - \int_{\theta_n}^{\theta}\lambda\,d\theta\right\}dc \qquad (3.27)$$

3.3 Inclusion of Salt Sieving in the Convective-Dispersive Transport Equation for Solutes

The existence of an osmotic gradient as a driving force on the liquid in soils and clays has been recognized for some time (Kemper and Rollins, 1966; Kemper and Letey, 1968; Groenevelt and Bolt, 1969). This phenomenon is usually attributed to the exclusion of anions from negatively charged surfaces of soil pores. The clay or soil then behaves as a "leaky" semi-permeable membrane. The effect of anion exclusion on flow of anions in soils has also been studied (Thomas and Swoboda, 1970; Krupp, Biggar and Nielsen, 1972). The contribution of osmosis* and anion exclusion to the simultaneous transport of salt and water in unsaturated soils under transient conditions has recently been explored by Bresler (1973, 1978). Bresler (1978) developed two separate equations to describe the rate of change of water content with time and the rate of change of salt concentration with time. It is interesting to note that the reflection coefficient σ (termed the "osmotic efficiency coefficient" in Bresler's paper) appears in the equation describing water movement whereas his equation describing the movement of salt omits the effects of salt-sieving, which is the counterpart of osmosis.

In this section of the study, basic equations in irreversible thermodynamics are used to develop the governing partial differential equation describing transient one-dimensional simultaneous transfer of salt and water. The objective in this study is to examine the movement of Cl^- during horizontal infiltration of KCl solution into a soil whose colloidal complex is saturated with Ca^{2+}. In this development, subscripts 1 and 2 will be used to refer to the salts KCl and $CaCl_2$ respectively.

The rate of entropy production (σ), or the dissipation function, $T\sigma$,(the rate of entropy production times the temperature), is equal to the sum of the products of the fluxes and forces in the system. The appropriate equation representing the dissipation function for the

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* movement of water due to salt concentration gradient in soil.

system under consideration is:

$$T\sigma = -\Sigma j_k \cdot \nabla\tilde{\mu}_k \tag{3.28a}$$

where T is the temperature (K)

σ is the rate of entropy production (kg m^{-1} s^{-3} K^{-1})

j_k is the flux of the component k (kg m^{-2} s^{-1})

$\tilde{\mu}_k$ is the total thermodynamic potential of component k (i.e. chemical potential plus external force fields (m^2 s^{-2})

Equation 3.28a is written for the system we are considering as:

$$T\sigma = -j_w \cdot \nabla\tilde{\mu}_w - j_{s1} \cdot \nabla\tilde{\mu}_{s1} - j_{s2} \cdot \nabla\tilde{\mu}_{s2} \tag{3.28b}$$

where subscripts w, s1 and s2 refer to water, salt 1 (KCl) and salt 2 ($CaCl_2$) respectively.

At constant temperature $\nabla\tilde{\mu}$ for water and solutes can be written as:

$$\nabla\tilde{\mu}_w = \bar{V}_w \nabla P + \nabla\mu^c{}_w \tag{3.29a}$$

$$\nabla\tilde{\mu}_{s1} = \bar{V}_{s1} \nabla P + \nabla\mu^c{}_{s1} \tag{3.29b}$$

$$\nabla\tilde{\mu}_{s2} = \bar{V}_{s2} \nabla P + \nabla\mu^c{}_{s2} \tag{3.29c}$$

where $\bar{V}_k$ is the specific volume of constituent k (volume of k/mass of k, m^3 kg^{-1})

$\mu^c{}_k$ is the concentration dependent part of the total thermodynamic potential $\tilde{\mu}$ (m^2 $s-^2$)

P is the pressure within the liquid phase (kg m^{-1} s^{-2}).

In equations 3.29a, 3.29b and 3.29c the gravity component of $\tilde{\mu}$ has been neglected and so any derivations using the equations are restricted to horizontal flow. Substitution of equations 3.29a, 3.29b and 3.29c into equation 3.28b yields:

$$T\sigma = -j_w(\bar{V}_w\nabla P + \nabla\mu_w) - j_{s1}(\bar{V}_{s1}\nabla P + \nabla\mu^c{}_{s1}) - j_{s2}(\bar{V}_{s2}\nabla P + \nabla\mu^c{}_{s2})$$

$$= -j^v\nabla P - j_w\nabla\mu^c{}_w - j_{s1}\nabla\mu^c{}_{s1} - j_{s2}\nabla\mu^c{}_{s2} \qquad (3.30a)$$

where j^v is the total volume flux (ms^{-1}) defined as

$$j^v = j_w\bar{V}_w + j_{s1}\bar{V}_{s1} + j_{s2}\bar{V}_{s2} \qquad (3.30b)$$

In neutral salt solutions the concentration dependent parts of the thermodynamic potential of the different components are connected via the Gibbs-Duhem equation:

$$\rho_w\ \nabla\mu^c{}_w + \rho_{s1}\ \nabla\mu^c{}_{s1} + \rho_{s2}\ \nabla\mu^c{}_{s2} = 0 \qquad (3.31)$$

where ρ_k is the bulk density of constitutent k (mass of k/volume of mixture; kg m^{-3}).

Equation 3.31 gives:

$$\nabla\mu^c_w = -\frac{\rho_{s_1}}{\rho_w}\nabla\mu^c_{s_1} - \frac{\rho_{s_2}}{\rho_w}\nabla\mu^c_{s_2}$$

which upon substitution into equation 3.30a gives

$$T\sigma = -j^v\nabla P + j_w\left[\frac{\rho_{s_1}}{\rho_w}\nabla\mu^c_{s_1} + \frac{\rho_{s_2}}{\rho_w}\nabla\mu^c_{s_2}\right] - j_{s_1}\nabla\mu^c_{s_1} - j_{s_2}\nabla\mu^c_{s_2}$$

$$= -j^v\nabla P - (j_{s_1} - v_w\rho_{s_1})\nabla\mu^c_{s_1} - (j_{s_2} - v_w\rho_{s_2})\nabla\mu^c_{s_2} \qquad (3.32a)$$

In equation 3.32a, v_w is the linear velocity of water (ms^{-1}). For the rest of the development, v_k is the linear velocity of constituent k. The flux j_k of constituent k is given by the relationship:

$$j_k = \rho_k v_k$$

Equation 3.32a therefore becomes:

$$T\sigma = -j^v\nabla P - \rho_{s_1}(v_{s_1} - v_w)\nabla\mu^c_{s_1} - \rho_{s_2}(v_{s_2} - v_w)\nabla\mu^c_{s_2} \qquad (3.32b)$$

The osmotic potential gradient may be defined as:

$$-\rho_w\nabla\mu^c_w = \sum_{k=s1,s2}\rho_k\nabla\mu^c_k = \phi_w\nabla\pi$$

The total osmotic pressure gradient ($\nabla\pi$) may now be split into two parts ($\nabla\pi = \nabla\pi_1 + \nabla\pi_2$), each part being the effect of the presence of one of the two salts. Then, according to Van't Hoff's law:

$$\nabla\pi_1 = n_1RT\nabla c_1 \text{ and } \nabla\pi_2 = n_2RT\nabla c_2$$

Thus,

$$T\sigma = -j^v\nabla P - \phi_w(v_{s1}-v_w)n_1RT\nabla c_1 - \phi_w(v_{s2}-v_w)n_2RT\nabla c_2 \tag{3.33}$$

In equation 3.33,

R is the gas constant in ergs per mole per °K.

T is the temperature (K).

c_k is the concentration of constituent k (moles m^{-3}). If c_k is measured in equivalents/m^3 of K^+ and Ca^{2+}, then n_k (the number of particles the salt will dissociate into) is 2 for salt 1 and 3 for salt 2.

ϕ_k is the volume fraction of constituent k (= $\rho_k\bar{V}_k$).

Therefore,

$$T\sigma = -j^v\nabla P - j_1^D n_1RT\nabla c_1 - j_2n_2RT\nabla c_2 \tag{3.34a}$$

or

$$T\sigma = -j^v\nabla P - j_1^D\nabla\pi_1 - j_2^D\nabla\pi_2 \tag{3.34b}$$

where

j_1^D and j_2^D are the diffusion flux of salt 1 and salt 2 respectively and are defined as

$$j_1^D = \phi_w(v_{s1} - v_w) \tag{3.35a}$$

$$j_2^D = \phi_w(v_{s2} - v_w) \tag{3.35b}$$

The dissipation function has been transformed from the expression as stated in equation 3.28 to the expression in equation 3.34a because the forces in the latter are more directly measurable.

Since the flux of constituent k is given by the relationship:

$j_k = \rho_k v_k$, equation 3.30b becomes:

$j^v = \rho_w v_w \bar{V}_w + \rho_{s1} v_{s1} \bar{V}_{s1} + \rho_{s2} v_{s2} \bar{V}_{s2}$ which

upon further substitution of the volume fraction of constituent k given by the relationship

$\phi_k = \rho_k \bar{V}_k$ yields:

$$j^v = \phi_w v_w + \phi_{s1} v_{s1} + \phi_{s2} v_{s2} \ .$$

Therefore,

$$\phi_w v_w = j^v - (\phi_{s1} v_{s1} + \phi_{s2} v_{s2}) \tag{3.36}$$

Substitute equation 3.36 into equations 3.35a and 3.35b.

$$j_1^D = \phi_w v_{s1} - [j^v - (\phi_{s1} v_{s1} + \phi_{s2} v_{s2})]$$

$$= (\phi_w + \phi_{s1})\, v_{s1} + \phi_{s2} v_{s2} - j^V \tag{3.37a}$$

$$j_2^D = \phi_s v_{s2} - [j^V - (\phi_{s1} v_{s1} + \phi_{s2} v_{s2})]$$

$$= (\phi_w + \phi_{s2})\, v_{s2} + \phi_{s1} v_{s1} - j^V \tag{3.37b}$$

The terms $\phi_{s2} v_{s2}$ and $\phi_{s1} v_{s1}$ in equations 3.37a and 3.37b appear to be necessary in order to account for the possibility that the two salts have a common anion (or cation), in particular when the diffusion flux is monitored according to the movement of that common ion. It should be pointed out that both $\phi_{s1} v_{s1}$ and $\phi_{s2} v_{s2}$ are very small in comparison to the other terms in the equations.

The transport equations for water and salt are now composed from equation 3.34b according to the following general guideline: every flux appearing in the dissipation equation is set to be a linear homogeneous function of every force appearing in that same equation. Thus:

$$j^V = -L_V \nabla P - L_{VD1} \nabla \pi_1 - L_{VD2} \nabla \pi_2 \tag{3.38a}$$

$$j_1^D = -L_{DV1} \nabla P - L_{D1} \nabla \pi_1 - L_{DD2} \nabla \pi_2 \tag{3.38b}$$

$$j_2^D = -L_{DV2} \nabla P - L_{DD1} \nabla \pi_1 - L_{D2} \nabla \pi_2 \tag{3.38c}$$

where L is called the phenomenological coefficient and represents the constant of proportionality between the flux and the force. L_V is directly related to the hydraulic conductivity, L_{VD} is the coefficient relating the flow of water conjugate to an osmotic pressure gradient (capillary osmosis) and L_{DV} is the salt sieving coefficient, that is the coefficient representing the movement of the solute relative to the solvent as a pressure gradient is applied in the absence of concentration gradients. In general, L_{ij} is a coupling coefficient relating flux of entity i due to the force conjugate to entity j.

At this stage, only the movement of salt 1 will be considered. Substitution of j^V from equation 3.38a into equation 3.37a gives:

$$j_1^D = (\phi_w + \phi_{s1})v_{s1} + \phi_{s2}v_{s2} - (-L_V\nabla P - L_{VD1}\nabla\pi_1 - L_{VD2}\nabla\pi_2)$$

Therefore,

$$(\phi_w + \phi_{s1})v_{s1} + \phi_{s2}v_{s2} = j_1^D - L_V\nabla P - L_{VD1}\nabla\pi_1 - L_{VD2}\nabla\pi_2 \qquad (3.39)$$

Substitute equation 3.38b into equation 3.39 for j_1^D:

$$(\phi_w + \phi_{s1})v_{s1} + \phi_{s2}v_{s2} = -L_{DV1}\nabla P - L_{D1}\nabla\pi_1 - L_{DD2}\nabla\pi_2 - L_V\nabla P - L_{VD1}\nabla\pi_1 - L_{VD2}\nabla\pi_2$$

Therefore,

$$(\phi_w + \phi_{s1})v_{s1} + \phi_{s2}v_{s2} = -(L_V + L_{DV1})\nabla P - (L_{D1} + L_{VD1})\nabla\pi_1 - (L_{DD2} + L_{VD2})\nabla\pi_2 \qquad (3.40)$$

As a first approximation, $-L_{DD2}\nabla\pi_2$ which is a second order interaction term and may be very small in magnitude in comparison with the other terms, is omitted.

$$(\phi_w + \phi_{s1})\ {}_{s1} + \phi_{s2}v_{s2} = -(L_V + L_{DV1})\nabla P - (L_{D1} + L_{VD1})\nabla\pi_1 - L_{VD2}\nabla\pi_2 \qquad (3.41)$$

Assuming that the semi-permeable properties of the medium are the same for salt 1 and salt 2, then $L_{VD1} = L_{VD2}$ and $\nabla\pi_1 + \nabla\pi_2 = \nabla\pi$, the total osmotic potential gradient. It must be pointed out that when two solutes are "different" (in dissociation or in size of particles), the semi-permeable properties of the soil with respect to the two solutes are different; for example, for a mixture of carbowax and KCl the semi-permeable properties of the medium will be very different for the two solutes.

Equation 3.41 with L_{VD1} set equal to L_{VD2} becomes:

$$(\phi_w + \phi_{S1})v_{s1} + \phi_{s2}v_{s2} = -(L_V + L_{DV1})\nabla P - L_{D1}\nabla\pi_1 - L_{VD1}\nabla\pi \qquad (3.42)$$

Multiply equation 3.42 through by c_1:

$$c_1(\phi_w+\phi_{s1})v_{s1} + c_1\phi_{s1}v_{s2} = -(L_V+L_{DV1})c_1\nabla P - L_{D1}c_1\nabla\pi_1 - L_{VD1}c_1\nabla\pi \qquad (3.43)$$

Equation 3.3b for unidimensional flow of salt and water may be written as:

$$q_s = -\theta D_s \nabla c - c K \nabla H \tag{3.44}$$

where ∇H is the hydraulic potential gradient (mm^{-1})

and K is the hydraulic conductivity (ms^{-1}).

Now comparing equations 3.43 and 3.44 it is observed that:

(i) $c_1[(\phi_w + \phi_{s1})v_{s1} + \phi_{s2}v_{s2}] \equiv q_s$

(ii) $-L_V c_1 \nabla P \equiv -c K \nabla H$

(iii) $-L_{D1} c_1 \nabla \pi_1 \equiv -\theta D_s \nabla c$

Therefore, in order to account for salt sieving effect, it is necessary to add terms equivalent to $(-L_{DV1} c_1 \nabla P - L_{VD1} c_1 \nabla \pi)$ to equation 3.44.

In order to characterise the permiselectivity of a porous sytem, one usually employs the reflection coefficient σ, which describes the salt sieving effect. It is defined by Staverman (1951) for flow of large solute molecules and solvent through an uncharged membrane as: the ratio of the diffusion flux due to the hydrostatic pressure gradient to the volume flux at zero osmotic potential gradient:

$$\sigma = - \left(\frac{j_1^D}{j^v}\right)_{\nabla\pi=0} \qquad (3.45a)$$

Therefore, setting $\nabla\pi_1$ and $\nabla\pi_2$ equal to zero in equations 3.38 a and 3.38b,

$$\sigma = - \left(\frac{j_1^D}{j^v}\right)_{\nabla\pi=0} = - \frac{L_{Dv1}}{L_V} \qquad (3.45b)$$

According to Onsager's principle of reciprocity, the phenomenological cross coefficients of equations 3.38a, 3.38b and 3.38c are equal and so from equation 3.45b

$$\sigma L_V = -L_{DV1} = -L_{VD1} \qquad (3.46)$$

For equation 3.44 to account for salt sieving effects, the complete form for our system under consideration is:

$$q_s = -\theta D_s \nabla c + \sigma L_V c \nabla\pi - cK\nabla H + \sigma L_V c \nabla P \qquad (3.47)$$

In equation 3.47, the first term on the righthand side accounts for dispersion, the second term accounts for osmosis, convection is accounted by the third term and salt sieving effect described by the fourth term. For the rest of this development the osmotic term will be left in π which will be converted to c by the use of Van't Hoff's law when the final equation is to be used to calculate D_s.

Also, $L_V = \frac{K(\theta)}{g\rho_w}$ (3.48a) and for horizontal flow,

$$H = P/g\rho_w \qquad (3.48b)$$

In equations 3.48a and 3.48b, ρ_w is density of water and g is the acceleration due to gravity (ms^{-2}). Therefore, the macroscopic form of equation 3.47 is:

$$q_s = -\theta D_s \frac{\partial c}{\partial x} + \frac{\sigma c K(\theta)}{g\rho_w} \frac{\partial \pi}{\partial x} - \frac{c K(\theta)}{g\rho_w} (1-\sigma) \frac{\partial P}{\partial x} \qquad (3.49)$$

[c is now in equivalents of Cl^- per m^3]

If we now define the soil moisture diffusivity $D(\theta)$ as

$$D(\theta) = \frac{K(\theta)}{g\rho_w} \frac{\partial P}{\partial \theta} ,$$

equation 3.49 becomes:

$$q_s = -\theta D_s \frac{\partial c}{\partial x} + \frac{\sigma c\ K(\theta)}{\rho_w g} \frac{\partial \pi}{\partial x} - (1-\sigma) c\ D(\theta) \frac{\partial \theta}{\partial x} \qquad (3.50)$$

M in the continuity equation for solute flow (equation 3.4) is defined for the case where salt sieving occurs as:

$$M = (\theta - \theta_{ex}) c_e \qquad (3.51a)$$

where c_e is the local equilibrium concentration.

Substitution of equation 3.51a into equation 3.4, gives

$$\frac{\partial}{\partial t}[(\theta-\theta_{ex})c_e] = -\partial q_s/\partial x \tag{3.51b}$$

In equations 3.51a and 3.51b, θ_{ex} is the volumetric water content of the exclusion zone where c=0 and M is the total quantity of solute in the bulk volume of soil. Substitution of equation 3.51b into equation 3.50 gives:

$$\frac{\partial(\theta c)}{\partial t} - \frac{\partial}{\partial t}(\theta_{ex}c) = \frac{\partial}{\partial x}[\theta D_s \frac{\partial c}{\partial x}] - \frac{\partial}{\partial x}(\frac{\sigma c K(\theta)}{g\rho_w}\frac{\partial \pi}{\partial x})$$

$$+ \frac{\partial}{\partial x}[(1-\sigma)cD(\theta)\frac{\partial \theta}{\partial x}]$$

As a first approximation, θ_{ex} is assumed constant, thus obtaining,

$$c\frac{\partial\theta}{\partial t} + \theta\frac{\partial c}{\partial t} - \theta_{ex}\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}[\theta D_s\frac{\partial c}{\partial x}] - \frac{\partial}{\partial x}(\frac{\sigma c K(\theta)}{g\rho_w}\frac{\partial \pi}{\partial x})$$

$$+ \frac{\partial}{\partial x}(cD(\theta)\frac{\partial\theta}{\partial x}) - \frac{\partial}{\partial x}[\sigma c D(\theta)\frac{\partial\theta}{\partial x}]$$

or,

$$c\frac{\partial\theta}{\partial t} + \theta\frac{\partial c}{\partial t} - \theta_{ex}\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}[\theta D_s\frac{\partial c}{\partial x}] - \frac{\partial}{\partial x}(\frac{\sigma c K(\theta)}{g\rho_w}\frac{\partial \pi}{\partial x})$$

$$+ c\frac{\partial}{\partial x}(D(\theta)\frac{\partial\theta}{\partial x}) + D(\theta)\frac{\partial\theta}{\partial x}\frac{\partial c}{\partial x}$$

$$- \frac{\partial}{\partial x}(\sigma c D(\theta)\frac{\partial\theta}{\partial x}) \tag{3.52}$$

The continuity equation for water flow is written as:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[D(\theta)\frac{\partial\theta}{\partial x}\right]$$

Therefore, the term $c\,\frac{\partial\theta}{\partial t}$ on the left hand side of equation 3.53 cancels $c\,\frac{\partial}{\partial x}\left[D(\theta)\,\frac{\partial\theta}{\partial x}\right]$ on the right hand side:

$$\frac{\theta\partial c}{\partial t} - \theta_{ex}\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[\theta D_s\frac{\partial c}{\partial x}\right] - \frac{\partial}{\partial x}\left(\frac{\sigma cK(\theta)}{g\rho_w}\frac{\partial\pi}{\partial x}\right)$$

$$+ D(\theta)\frac{\partial\theta}{\partial x}\frac{\partial c}{\partial x} - \frac{\partial}{\partial x}\left[\sigma cD(\theta)\frac{\partial\theta}{\partial x}\right) \qquad (3.53)$$

Let $\lambda = xt^{-1/2}$ so that $\partial\lambda/\partial x = t^{-1/2}$, $\partial\lambda/\partial t = -\frac{\lambda}{2}t^{-1}$.

Substitution of λ into equation 3.53 gives:

$$-\frac{\theta\lambda}{2}\frac{dc}{d\lambda} + \frac{\lambda\theta_{ex}}{2}\frac{dc}{d\lambda} = \frac{d}{d\lambda}\left[\theta D_s\frac{dc}{d\lambda}\right] - \frac{d}{d\lambda}\left(\frac{\sigma cK(\theta)}{g\rho_w}\frac{d\pi}{d\lambda}\right)$$

$$+ D(\theta)\frac{d\theta}{d\lambda}\frac{dc}{d\lambda} - \frac{d}{d\lambda}\left(\sigma cD(\theta)\frac{d\theta}{d\lambda}\right) \qquad (3.54)$$

It is necessary at this stage to derive an approximate relationship between σ and concentration of Cl^- in solution, c, or water content θ in order to estimate σ. Substitution of the diffusion flux $j_1^D = \frac{j_s}{c_e} - j^v$, into equation 3.45b yields

$$\sigma = -\left[\frac{j_{s1}/c_e - j^v}{j^v}\right]_{\nabla\pi=0}$$

where c_e is the local equilibrium concentration.

$$\sigma = \left[1 - \frac{j_{s1}}{j^v c_e}\right]_{\nabla\pi=0}$$

But $$c_m = \left(\frac{j_{sl}}{j_v}\right)_{\nabla\pi=0}$$

where c_m is the mean local concentration.

Therefore,

$$\sigma = 1 - \frac{c_m}{c_e} \tag{3.55}$$

Alternatively, relation 3.55 is derived by considering that at the inlet end of our soil column, the equilibrium concentration is known ($c_{ei} = 1.0$) because the liquid there is directly in contact with an "equilibrium pool" (i.e. the solution in the inlet compartment). c_m is also measured for the first section of the soil column and so σ at $\lambda=0$ can be estimated. At some position λ^*, even though the equilibrium concentration is not known, the moisture content θ^* is known. Now consider figure 3.1 where A represents the surface of a soil pore, b_{ex} is the thickness of the exclusion layer where $c=0$ and b is the thickness of the film of water on the surface. Then

$$\sigma = \frac{b_{ex}}{b} = \frac{\theta_{ex}}{\theta} \tag{3.56}$$

Also,

$$c_m = \frac{c_e(b - b_{ex})}{b}$$

Therefore,

Figure 3.1: Schematic diagram indicating the exclusion zone, thickness of film of water and equilibrium concentration.

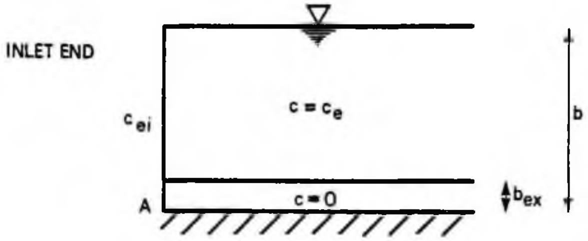

Figure 3.1

$$\frac{c_m}{c_e} = 1 - \frac{b_{ex}}{b}$$

and $$\sigma = \frac{b_{ex}}{b} = 1 - \frac{c_m}{c_e} \qquad (3.57)$$

which is similar to equation 3.55. Since c_{ei} is known for the inlet section, and σ at $\lambda=0$ is calculated using equation 3.57, θ_{ex} (assumed constant) can be estimated by substituting the σ calculated for $\lambda=0$ into equation 3.56. Thus at position λ^*

$$\sigma(\lambda^*) = \frac{\theta_{ex}}{\theta} \qquad (3.58)$$

Designating $\theta D_s \frac{dc}{d\lambda} = y$, equation 3.54 becomes

$$\frac{dy}{d\lambda} = \frac{\lambda\theta_{ex}}{2}\frac{dc}{d\lambda} - \frac{\theta\lambda}{2}\frac{dc}{d\lambda} + \frac{d}{d\lambda}\left(\frac{\sigma c K(\theta)}{g\rho_w}\frac{d\pi}{d\lambda}\right) - D(\theta)\frac{d\theta}{d\lambda}\frac{dc}{d\lambda}$$

$$+ \frac{d}{d\lambda}\left(\sigma c D(\theta)\frac{d\theta}{d\lambda}\right)$$

Multiply through by $d\lambda$ and integrate, noting that the initial and boundary conditions formulated in equations 3.20a and 3.20b imply that at $\theta = \theta_n$, $c = c_n$, and $\frac{d\theta}{d\lambda} = 0$, $\frac{dc}{d\lambda} = 0$ and hence $y_n = 0$. Thus,

$$y\Big|_{y_n}^{y} = \frac{\theta_{ex}}{2}\int_{c_n}^{c}\lambda dc - \frac{1}{2}\int_{c_n}^{c}\theta\lambda dc + \frac{\sigma c K(\theta)}{g\rho_w}\frac{d\pi}{d\lambda} - \int_{c_n}^{c} D(\theta)\frac{d\theta}{d\lambda}dc + \sigma c D(\theta)\frac{d\theta}{d\lambda}$$

It follows that,

$$y = \frac{1}{2}\int_{c_n}^{c} (\theta_{ex}\lambda - \theta\lambda - 2D(\theta)\,\frac{d\theta}{d\lambda})\,dc + \frac{\sigma cK(\theta)}{g\rho_w}\,\frac{d\pi}{d\lambda} + \sigma cD(\theta)\,\frac{d\theta}{d\lambda}$$

Therefore,

$$D_s = \frac{d\lambda}{dc}\,\frac{1}{\theta}\,[\,\frac{1}{2}\int_{c_n}^{c} (\theta_{ex}\lambda - \theta\lambda - 2D(\theta)\,\frac{d\theta}{d\lambda})\,dc + \frac{\theta_{ex}cK(\theta)}{g\rho_w}\,\frac{dc}{d\lambda} + \frac{\theta_{ex}cD(\theta)}{\theta}\,\frac{d\theta}{d\lambda}\,] \qquad (3.59)$$

Equation 3.59 was modified and solved using a computer program written in System 360 CSMP language (see figure 4.8 and section 4.9.4).

3.4 Dispersion During Vertical Infiltration

Assuming unidimensional flow during vertical infiltration, the flow velocity, v, is given by:

$$v = K(\theta) - D(\theta)\,\frac{\partial\theta}{\partial z} \qquad (3.61)$$

where z is the vertical space coordinate taken positive downward. Substitution of equation 3.10 (with z instead of x) into 3.61 gives the equation describing the distribution of water content with time for vertical flow:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\,[D(\theta)\,\frac{\partial\theta}{\partial z}] - \frac{\partial K(\theta)}{\partial z} \qquad (3.62)$$

The following initial and boundary conditions apply:

$$\theta = \theta_n, \; z > 0, \; t = 0 \tag{3.63a}$$

$$\theta = \theta_o, \; z = 0, \; t \geq 0 \tag{3.63b}$$

Substitution of equation 3.61 into 3.15a (with z instead of x) yields the equation describing the rate of change of concentration of nonreactive solute with time for vertical flow:

$$\theta \frac{\partial c}{\partial t} = \frac{\partial}{\partial z} [\theta D_s(\theta) \frac{\partial c}{\partial z}] - [K(\theta) - D(\theta) \frac{\partial \theta}{\partial z}] \frac{\partial c}{\partial z}$$

or

$$\theta \frac{\partial c}{\partial t} = \frac{\partial}{\partial z} [\theta D_s(\theta) \frac{\partial c}{\partial z}] + D(\theta) \frac{\partial \theta}{\partial z} \frac{\partial c}{\partial z} - K(\theta) \frac{\partial c}{\partial z} \tag{3.64}$$

The initial condition for the solute is:

$$c = c_n, \; z > 0, \; t = 0 \tag{3.65a}$$

As discussed by Smiles et al. (1978) two forms of boundary conditions are possibly appropriate, namely the constant concentration boundary condition:

$$c = c_o, \; z = 0, \; t > 0 \tag{3.65b}$$

or the flux boundary condition:

$$- \theta D_s(\theta) \frac{\partial c}{\partial z} = v(c_o - c), \; z = 0, \; t > 0 \tag{3.65c}$$

As shown by Philip (1957) and later used by Elrick et al. (1979), equations 3.62 and 3.64 rewritten with z as the dependent variable are of the form:

$$-\frac{\partial z}{\partial t} + \frac{\partial K(\theta)}{\partial \theta} = \frac{\partial}{\partial \theta}\left[\frac{D(\theta)}{\partial z/\partial \theta}\right] \qquad (3.66)$$

and

$$-\theta\frac{\partial z}{\partial t} + K(\theta) - \frac{D(\theta)}{\partial z/\partial \theta} = \frac{\partial}{\partial c}\left[\frac{\theta D_s(\theta)}{\partial z/\partial c}\right]. \qquad (3.67)$$

Both equations 3.66 and 3.67, subject to conditions 3.63a, 3.63b, 3.65a, 3.65b, have solutions in power series of the form:

$$z(\theta) = \lambda(\theta)t^{1/2} + \chi_w(\theta)t + \psi_w(\theta)t^{3/2} + \omega_w(\theta)t^2 + \ldots \qquad (3.68)$$

$$z(c) = \lambda(c)t^{1/2} + \chi_s(c)t + \psi_s(c)t^{3/2} + \omega_s(c)t^2 + \ldots \qquad (3.69)$$

Details of the mathematical treatment for obtaining the coefficients λ, χ, ψ, ω etc. as given by Philip (1957) and Elrick et al. (1979) are provided in Appendices A and B. The resultant ordinary differential equations for λ, χ, ψ and ω are summarized in Table 3.1.

In equations 3.72 through to 3.77 it is observed that χ, ψ and ω are the dependent variables and that θ or c is the independent variable. Consequently it is appropriate to designate χ, ψ and ω for water flow with a subscript, w, (thus we have χ_w, ψ_w and ω_w) and to use subscript 's' for salt flow, i.e., χ_s, ψ_s and ω_s. It is pertinent to mention that $\chi_w(\theta)$ and $\chi_s(c)$ are not the same. Also, $\psi_w \neq \psi_s$ and $\omega_w \neq \omega_s$. Physically this must be so since the salt front always lags behind the water front.

* TABLE 3.1. Ordinary Differential Equations for Water and Solute Transport

Variable	Water		Solute	
λ	$-\frac{\lambda}{2} = \frac{d}{d\theta}\,[D(\theta)\frac{d\theta}{d\lambda}]$	(3.70)	$\frac{\theta\lambda}{2} + D(\theta)\,\frac{d\theta}{d\lambda} = -\frac{d}{dc}\,[\theta D_s(\theta)\,\frac{dc}{d\lambda}]$	(3.71)
χ	$\chi_w = \frac{d}{d\theta}\,[P(\theta)\,\frac{d\chi_w}{d\theta}] + \frac{dK(\theta)}{d\theta}$	(3.72)	$\theta\chi_s - [P(\theta)\,\frac{d\chi_w}{d\theta} + K(\theta)] = \frac{d}{dc}[P_s(\theta)\,\frac{d\chi_s}{dc}]$	(3.73)
ψ	$\frac{3}{2}\psi_w = \frac{d}{d\theta}[P(\theta)\,\frac{d\psi_w}{d\theta} - Q(\theta)]$	(3.74)	$\frac{3}{2}\theta\psi_s - [P(\theta)\,\frac{d\psi_w}{d\theta} - Q(\theta)] = \frac{d}{dc}[P_s(\theta)\,\frac{d\psi_s}{dc} - Q_s(\theta)]$	(3.75)
ω	$2\omega_w = \frac{d}{d\theta}\,[P(\theta)\,\frac{d\omega_w}{d\theta} - R(\theta)]$	(3.76)	$2\theta\omega_s - [P(\theta)\,\frac{d\omega_w}{d\theta} - R(\theta)] = \frac{d}{dc}\,[P_s(\theta)\,\frac{d\omega_s}{dc} - R_s(\theta)]$	(3.77)
	$P(\theta) = D(\theta)\,[\frac{d\theta}{d\lambda}]^2$	(3.78)	$P_s(\theta) = \theta D_s(\theta)\,[\frac{dc}{d\lambda}]^2$	(3.79)
	$Q(\theta) = D(\theta)\,\frac{d\theta}{d\lambda}(\frac{d\chi_w}{d\lambda})^2$	(3.80)	$Q_s(\theta) = \theta D_s(\theta)\,\frac{dc}{d\lambda}(\frac{d\chi_s}{d\lambda})^2$	(3.81)
	$R(\theta) = Q(\theta)\,[2\,\frac{d\psi_w}{d\chi_w} - \frac{d\chi_w}{d\lambda}]$	(3.82)	$R_s(\theta) = Q_s(\theta)\,[2\,\frac{d\psi_s}{d\chi_s} - \frac{d\chi_s}{d\lambda}]$	(3.83)

* From Elrick *et al*. (1979).

The theory presented in this chapter was tested experimentally using two clay soils which have relatively high cation exchange capacities. Chapter 4 which follows, describes in detail the experiments conducted. It is, however, pertinent at this stage to introduce briefly the experiments conducted to test the theory presented for (a) transport of solutes which interact with the soil matrix, (b) flow systems where anion exclusion occurs and (c) for vertical movement of water and chloride in soils.

Preliminary experiments were conducted to:

(i) ascertain if the assumption of instantaneous equilibrium between the solid and solution phases is valid;

(ii) determine the adsorption isotherm for these soils;

(iii) verify the method used to estimate the concentration of K^+ in solution during the horizontal infiltration experiments, and

(iv) determine the soil moisture characteristic curves for sorption and desorption.

Horizontal infiltration experiments were conducted to obtain $\theta(\lambda)$ and $c(\lambda)$ data which were used to calculate $D_s(\theta)$. The converse problem of predicting $c(\lambda)$ from the calculated $D_s(\theta)$ data was also done using C.S.M.P. Also, the theory developed for the calculation of $D_s(\theta)$ in a flow system where anion exclusion occurs, was tested. Lastly, using the theory developed for vertical infiltration and input data $\theta(\lambda)$, $c(\lambda)$ (from the horizontal infiltration experiments) and $K(\theta)$ data, both water and chloride content profiles for vertical infiltration of water and solutes, were predicted.

CHAPTER 4

MATERIALS AND METHODS

4.1 Soils

The soils used in this study are:

(i) the Akuse clay loam which is a tropical black clay normally found under coastal savannah vegetation in Ghana. This soil is usually developed over basic gneiss (hornblende gneiss) and occurs on very gentle upland topography. It is dark grey to black, is sticky and plastic when wet but becomes hard and compact with cracks when dry. The dominant clay mineral is smectite (Oteng, 1976). Samples from 0-15 cm depth were used;

(ii) the Brookston clay loam, an Orthic humic gleysol, is a poorly drained member of the Huron catena. This soil is usually developed over clay rich glacial till. The dominant clay mineral in this soil is illite. Samples of 0-15 cm depth, collected from Essex county in Southern Ontario, were used in this study;

(iii) Caledon fine sandy loam, a grey brown podzolic from East half of concession 1,Lot number 30,of Erin Township in Southern Ontario was used to check the concentration measurements from the chloride analysis. This soil is dark greyish brown and usually developed on fine sands overlying coarse gravel. Samples from 0-15 cm depth were used.

Pertinent physical and chemical characteristics of these soils are given in Table 4.1.

TABLE 4.1. Some chemical and physical characteristics of the soils used.

	CEC	Exchangeable cations				pH in 0.01M $CaCl_2$ 1:2	% Organic Carbon	Particle size analysis			Saturated Hydraulic Conductivity ms^{-1}
	me/ 100 g	Ca^{++} me/ 100 g	Mg^{++} me/ 100 g	K^{+} me/ 100 g	Na^{+} me/ 100 g			% Sand	% Silt	% Clay	
Akuse	29.24	28.09	0.069	0.23	0.67	6.35	1.19	47.98	18.31	33.71	1.54×10^{-5}
Brookston	26.16	19.0	5.33	0.51	0.22	6.10	3.19	17.0	48.0	35.0	4.31×10^{-6}

4.2 Saturation of exchange complex of soils with calcium

One kilogram of sieved soil was placed in a Buchner funnel. Two litres of 0.5M calcium nitrate adjusted to pH 7.0 were leached through the soil very slowly, stopping the flow periodically by fitting a rubber stopper to the outlet of the funnel, in order to ensure effective exchange of cations. Samples of the effluent were collected after the last portion of the calcium nitrate solution had been allowed to saturate the soil overnight. The effluent collected was analysed for potassium to ascertain if most of the local exchangeable K^+ were replaced by calcium. The soil was then washed with two litres of deionised water after which it was air-dried, ground and sieved to pass through a 0.25 mm sieve with square holes (wire woven).

4.3 Time of equilibration experiments

The purpose of this experiment was to determine the time required for equilibrium conditions to be established between the quantity of K^+ adsorbed by soil and K^+ in solution in order to allow sufficient time for equilibrium to be achieved in the 'batch-shaking' procedure used for the adsorption isotherm* determination. In addition, it was necessary to ascertain if the assumption of instantaneous equilibrium used to develop equation 3.8b is sufficiently justified.

Five grams of soil (in triplicate) were placed in 15 ml plastic

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* An adsorption isotherm is the relation between the amount of solute per unit weight adsorbed by the porous material in equilibrium with concentration of the same species of solute in solution.

centrifuge tubes. Five millilitres solution of KCl adjusted to pH 7.0 and containing 1.0 m.e. K^+ was added to each tube and equilibrated on a reciprocating shaker for the following time periods: 5, 10, 15, 30, 60, 120 and 180 minutes. At the end of each shaking period, the set of tubes for that treatment was centrifuged for 5 minutes and the supernatant solution decanted and stored for analysis of K^+ using the atomic absorption spectrophotometer.

4.4 Determination of Adsorption Isotherms

Quantitative determination of potassium adsorption by soils from solution is essential to an understanding of the contribution of adsorption to the transport of potassium in soils. The conventional method, "batch equilibration method", which involves measurement of concentration changes in a solution of known volume after shaking with an adsorbent of known weight was used.

Five grams of the sieved Ca-saturated soil were weighed into a 15 ml plastic centrifuge tube. Five millilitres of 0.001M, 0.002M, 0.003M, 0.004M, 0.005M, 0.006M, 0.008M, 0.01M, 0.02M, 0.03M, 0.04M, 0.06M, 0.08M, 0.1M, 0.2M, 0.4M, 0.6M, 0.8M and 1.0M KCl solution adjusted to pH 7.0 were added to each tube and equilibrated for three hours on a reciprocating shaker. The tubes were then centrifuged for 5 minutes and the supernatant analysed for both K^+ using the atomic absorption spectrophotometer and Cl^- using a method similar to the Technicon Autoanalyzer Industrial method no. 99-70W. The concentrations of K^+ and Cl^- in the original stock solutions were analysed and by difference between this measured concentration of the stock solution and the concentration of the solution after equilibration, the amount of K^+ or Cl^- adsorbed per gram of soil was calculated and plotted against the equilibrium concentration.

4.5 High energy moisture characteristics*

A Buchner funnel with a sintered plate (porosity 4) connected by flexible tubing to a hanging column of water and a horizontal 10 ml burette was set up with the surface of the sintered plate at a matric potential of -120.0 cm H_2O. The initial volume of water in the horizontal burette was noted. A known mass of soil (which was subsequently used in the infiltration experiments), of known moisture content was poured into the funnel and tapped gently to a predetermined volume so that the bulk density at packing was also known. The horizontal burette ensured that sorption occurred at a constant matric potential of -120.0 cm. When there was no further uptake of water by the soil (i.e. when the meniscus of water in the horizontal burette was constant) the volume of water absorbed was read off. The volumetric moisture content of the soil at this matric potential was obtained by adding the volume of water adsorbed to the original water in the soil before packing into the funnel and expressing it as a ratio to the total volume into which the soil was packed. The complete sorption cycle from a moisture potential of -120.0 cm H_2O to moisture potential of zero was thus obtained by determining the equilibrium moisture content for successive 20 cm reductions in the height of the hanging column (i.e. 20 cm increases in matric potential). Once at

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* High energy refers to matric potentials from slightly greater than zero to approximately -120 cm H_2O.

matric potential of zero (measured relative to the middle of the soil sample) the draining cycle was determined on the same sample by lowering the hanging column in 20 cm steps. A check on cumulative quantities of water taken up and subsequently released by the soil was obtained by sampling at matric potential of -120 H_2O.

4.6 Determination of Hydraulic Conductivity

The saturated hydraulic conductivity of the Ca-saturated soils used in the horizontal infiltration experiments was determined with a constant head permeameter.

The unsaturated hydraulic conductivity, $K(\theta)$, was obtained from the sorption moisture characteristic curve and the moisture diffusivity data obtained from horizontal infiltration experiments through the relationship

$$K(\theta) = D(\theta) \Big/ \frac{\partial h}{\partial \theta} \tag{4.1}$$

where D is the soil water diffusivity and $\partial h/\partial\theta$ is the slope of the moisture characteristic curve.

The computation of the $K(\theta)$ values was done with a computer program written in system 360 CSMP (see Appendix C1 for description).

4.7 Chemical Analyses

Cation exchange capacity and exchangeable cations were determined by standard methods (Chapman, 1965). Organic matter was determined by the method of Walkley-Black (1934) and pH in 0.01M $CaCl_2$ by the method of Peech (1965).

4.8 Horizontal Infiltration Experiments

The infiltration column (Figure 4.1) used in the present study is similar to that used by Elrick *et al*. (1979). It consisted of a cylinder (A), 0.45 m long and an internal diameter 0.0285 m which was assembled from lucite sections made up of two lengths (refer to fig. 4.2 and D and F of fig. 4.3). The inlet region up to about the middle of the column was made of sections 0.0199 m long (fig. 4.3D) and from the middle to the end made of sections 0.0098 m long (fig. 4.3F). The first section of the column (fig. 4.3E) has two entry ports (one for entry of solution and the other to aid in the escape of air). Also a glass bead base (approximately 0.002 m thick) was provided in this section to facilitate the establishment of the boundary condition at x=0.

The second section in the column (fig. 4.3D) has a groove in which a 0.035 m (internal diameter) lurene O-ring is embedded to ensure a watertight seal. In order to ensure proper alignment of the sections, an acrylic rod in addition to two small rods (fig. 4.2) were used. These rods were removed once alignment of the sections was obtained and the frame made to hold these sections has securely been tightened (fig. 4.1).

Uniformity of packing of the column of soil was achieved by pouring the soil into the column evenly and tapping at the same time as the soil was being poured.

With the Akuse soil, two initial moisture contents were investigated, namely air-dry water content of 0.05 and a moistened soil of water content $\theta = 0.10$. Only the moistened soil of water content 0.12 was investigated in the case of the Brookston soil whilst the Caledon sand used to check the concentration analysis of chloride had an initial moisture content of 0.001. All the experiments were carried out in a laboratory in which the temperature varied between 21 and 23 C.

The most critical phase of the experiment was the start. Initially, the burette (B) was raised to the same level as the top of the horizontal column of soil. The burette was then opened and the stop watch started simultaneously. After about 30 s, the initial positive inflow head was lowered to approximately -1 mbar and at the same time the port for the escape of air was closed.

The infiltrating solution in all experiments was 1.0M KCl. The cumulative volume of solution as well as the distance to the wetting front was recorded as a function of the square root of time as an initial check on the preservation of similarity with regard to water flow. Data were obtained from experiments terminated at different elapsed times.

At the end of each infiltration experiment, the burette was closed and the final time recorded quickly. The bolts securing the frame were then loosened and with a small wooden plank placed on top of the column, it was knocked down thus slicing the column into sections. The moist soil from each section was quickly weighed in tared moisture dishes and then divided into two subsamples, half of which was used for gravimetric moisture content determination and then for the chloride determination. This initial weight of the wet soil in each section was used to calculate the oven dry equivalent of the soil in each section for the bulk density calculation, once the moisture content on weight basis was obtained on half of the sample from each section.

The other half of the wet soil from each section was weighed into a tared 15 ml centrifuge tube and used for the determination of concentration of potassium in solution during the infiltration experiment.

4.8.1 Determination of concentration of K^+ in solution during the infiltration experiment

Since the water content distribution of the horizontal column of soil was, for most of the sections, drier than saturation water content, it was not possible to directly determine the concentration of K^+ in solution

FIGURE 4.1

Set up for the Horizontal Infiltration Experiments

(see text for description)

Legend:

A	Horizontal column of soil
B	10 ml burette

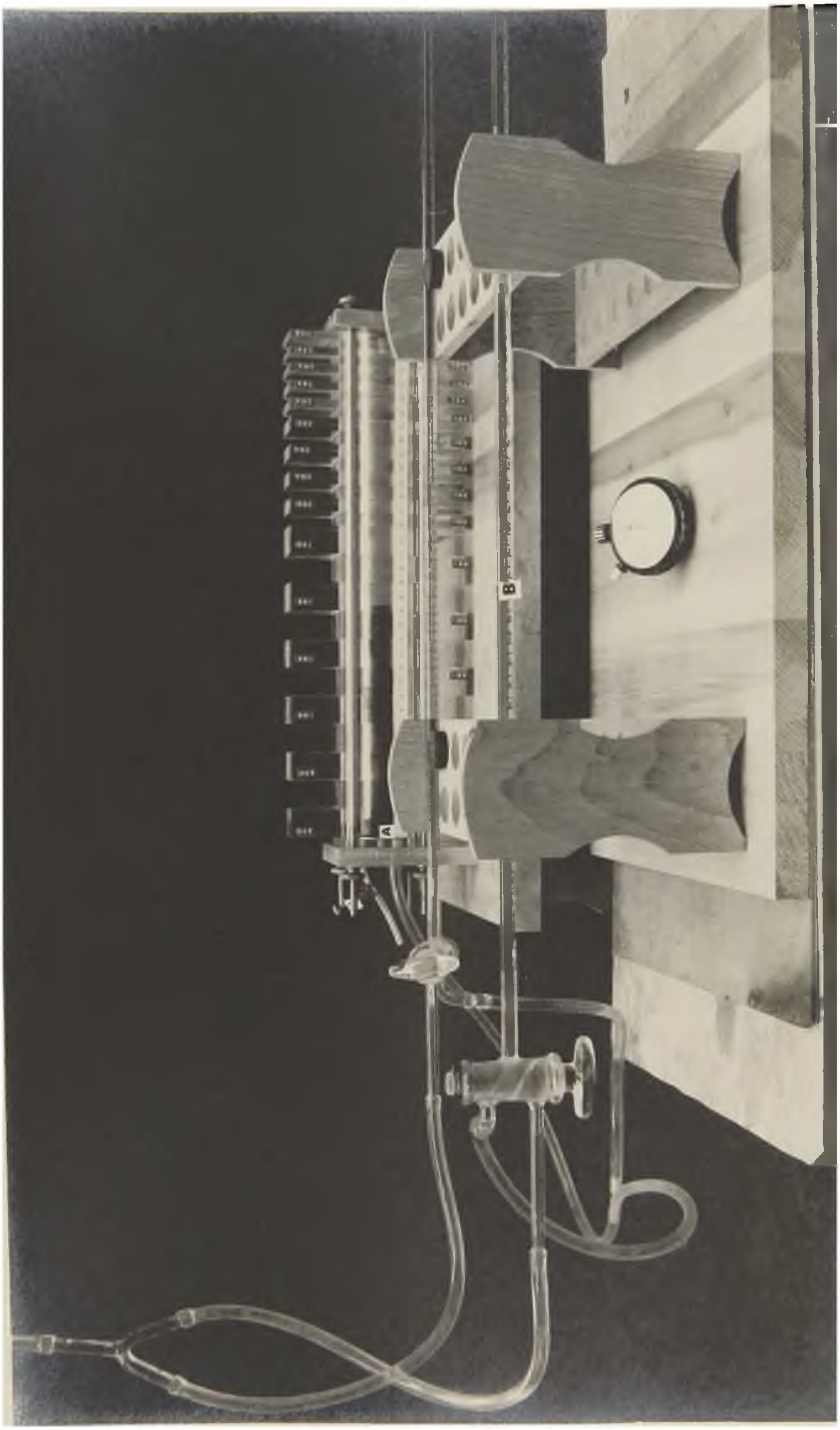

A
B

FIGURE 4.2

Some of the Sections Used for the Soil Column

An acrylic rod is used to ensure good alignment of the sections.

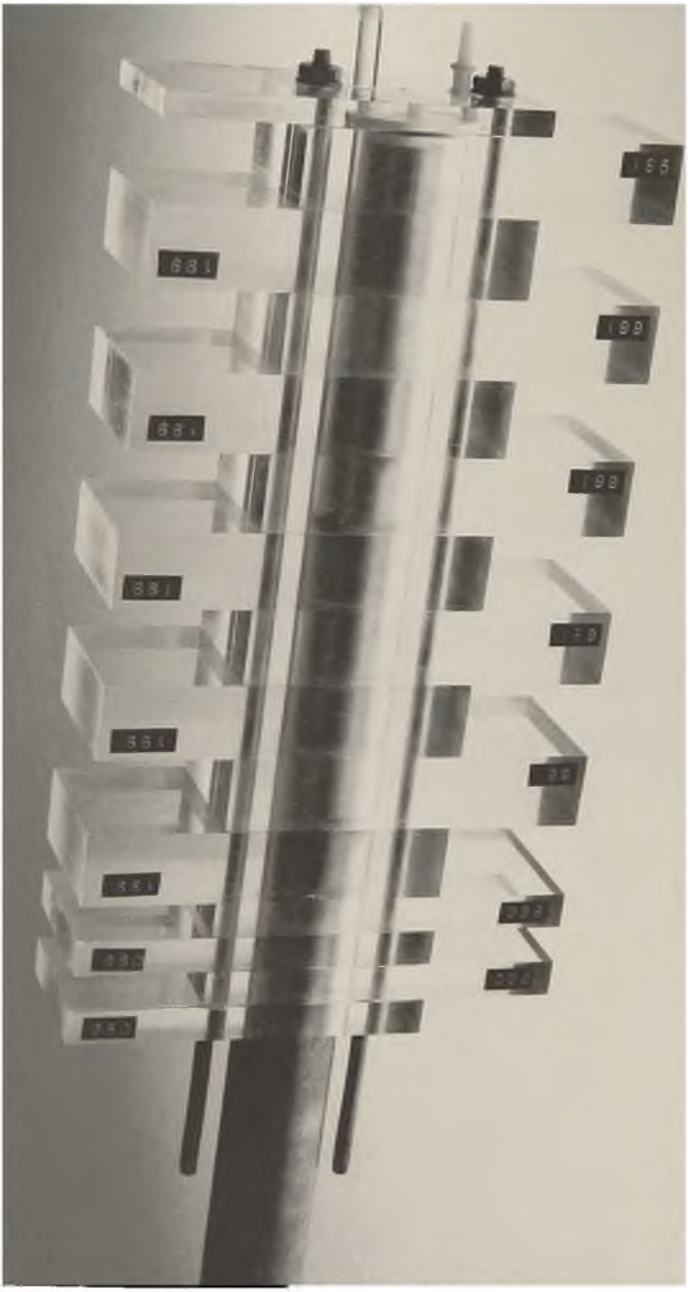
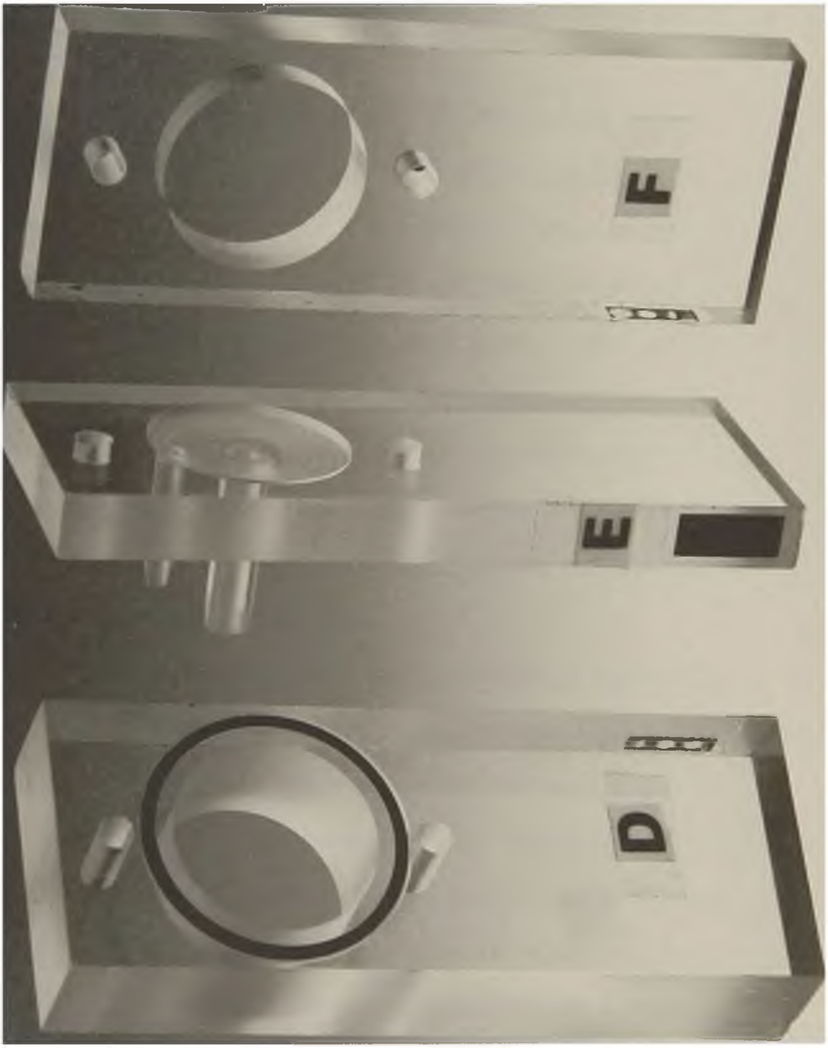


FIGURE 4.3

D: Lucite section with an O-ring to avoid leakage near the inlet end where soil is near saturation.

E: Inlet section showing the inlet tube and the air vent.

F: A thin section.


F
E
D

by extracting the soil solution through centrifugal filtration as was done, for example, by Soon and Miller (1977). A method was therefore developed to estimate the concentration of K^+ in solution during the horizontal infiltration experiment.

The weighed half of the moist soil from each section of the soil column was equilibrated with 5.0 ml of 0.5M KCl solution on a reciprocating shaker for 3 hours, after which the contents of each tube were centrifuged. The supernatant solution was then stored for determination of K^+ using Atomic Absorption Spectrophotometer. The concentration of K^+ in solution was then estimated from this equilibrium solution.

The theoretical consideration for the estimation of the concentration of K^+ in solution is as follows: consider a horizontal column which has been sectioned at the end of an infiltration experiment with KCl as the infiltrating solution (fig. 4.4).

The analysis which follows holds whether a sub-sample of the section was used or all the moist soil in the section was used. For simplicity, we will consider the case where the whole wet soil in each section was used. There is in each section, therefore, Ma_i which represents K^+ adsorbed on colloid during infiltration and the native K^+ (meq) and Ms_i, representing quantity of K^+ in solution (meq) during infiltration. Let us equilibrate each section with a known volume (say 5 ml) of a KCl solution whose concentration is higher than that of the soil solution after infiltration (an estimate of the concentration of KCl to use in this second equilibration may be obtained from the adsorption isotherm). We now have in the system Ma_e which represents the quantity of K^+ adsorbed during equilibration with the new solution of KCl (meq)

Figure 4.4: Schematic diagram of part of a sectioned column of soil.

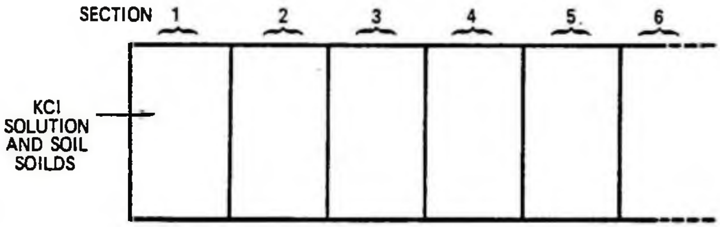


Figure 4.4

and Ms_e representing the quantity of K^+ in solution after the second equilibration (meq). Let M_e represent the amount of K^+ in the original volume of solution used for the second equilibration. The total quantity (meq) of K^+ adsorbed in both the infiltration experiment, the second equilibration and the native K^+ on the soil before the infiltration experiment are therefore represented by the sum of Ma_i and Ma_e which may be given the symbol Ma_{ie}. In this notation, 'a' stands for adsorbed, 'i' for infiltration, 's' for solution and 'e' for equilibration with another concentration.

The mass balance for this system then is given by

$$Ma_i + Ms_i + M_e = Ma_{ie} + Ms_e \tag{4.2a}$$

which for convenience may be written as

$$Ma_i + Ms_i = Ma_{ie} + Ms_e - M_e \tag{4.2b}$$

Now, in order to calculate Ms_i and hence the concentration of K^+ in solution during the infiltration experiment, Cs_i, we represent:

(i) the meq. K^+ adsorbed per gram of soil during the infiltration experiment and the meq. K^+ originally on the soil before infiltration, by Sa_i

$$Sa_i = \frac{Ma_i}{\text{Mass of soil solids}} \quad (\text{me/g}) \tag{4.3}$$

(ii) the meq. K^+ in equilibrium solution per litre of solution associated with Sa_i, by Cs_i

$$Cs_i = \frac{Ms_i}{\underset{y\ cm^3}{\text{Volume of solution (in sample say}}\text{)} \times 10^{-3}} \quad (\text{me}/1) \qquad (4.4)$$

(iii) the meq. K^+ in the adsorbed phase per gram soil after both infiltration and subsequent equilibration with another KCl solution of different concentration, by Sa_{ie}

$$Sa_{ie} = Ma_{ie}/\text{Mass of soil solids} \quad (\text{me/g}) \qquad (4.5)$$

(iv) the meq. K^+ in solution per litre after the equilibration with another KCl solution, by Cs_{ie}

$$Cs_{ie} = Ms_{ie}/\underset{\text{(i.e. 5+y)}}{\text{total volume of solution}} \times 10^{-3} \quad (\text{me}/1) \qquad (4.6)$$

Cs_{ie} is measured using the Atomic Absorption Spectrophotometer, and therefore Ms_{ie} may be obtained from equation 4.6. In addition to equations 4.2a to 4.6, we require the equation for the adsorption isotherm which in this study was given by a quadratic equation in the logarithmic form (equation 3.24) in order to solve the six equations with six unknowns.

Using equation 3.24 and the calculated Cs_{ie} from equation 4.6, we obtain Sa_{ie} and hence Ma_{ie} by substitution into equation 4.5. Since M_e is known, the righthand side ofthe mass balance equation 4.2b is known and may be represented by E.

Thus $Ma_i = E - Ms_i$ (4.7)

For the infiltration experiment, equation 3.24 may be written as

$$Sa_i = 10^{[-k_1 \log^2 Cs_i + k_2 \log Cs_i - k_3]}$$ which upon further substitution from equations 4.3 and 4.4 yields

$$\frac{Ma_i}{\text{Mass of soil solids}} = 10^{\left[-k_1 \log^2\left(\frac{Ms_i}{\text{Volume of solution} \times 10^{-3}}\right) + k_2 \log\left(\frac{Ms_i}{\text{Volume of solution} \times 10^{-3}}\right) - k_3\right]} \qquad (4.8)$$

Substituting for Ma_i on the lefthand side of equation 4.8 from equation 4.7 we obtain

$$\frac{E-Ms_i}{\text{Mass of soil solids}} = 10^{\left[-k_1 \log^2\left(\frac{Ms_i}{\text{Volume of solution} \times 10^{-3}}\right) + k_2 \log\left(\frac{Ms_i}{\text{Volume of solution} \times 10^{-3}}\right) - k_3\right]} \qquad (4.9)$$

Equation 4.9 is an implicit equation and was solved for Ms_i by an iterative procedure facilitated by a programmable calculator. Once a value for Ms_i was obtained, it was substituted into equation 4.4 to get Cs_i, the concentration of K^+ in solution during the infiltration experiment.

The assumptions inherent in this method of estimating the concentration of K^+ in solution during horizontal infiltration are that,

(i) equilibrium or pseudoequilibrium conditions exist between the quantity of solute adsorbed and the concentration in the solution phase such that the equilibrium adsorption isotherm is applicable;

(ii) the adsorption isotherm is unique when only the adsorption process is considered so that when the concentration in solution is increased through the second equilibration with fresh solution of KCl of known concentration, the new equilibrium that is established follows the original adsorption isotherm curve; and

(iii) the adsorption isotherm curve is not influenced by moisture content so that the equation for the adsorption isotherm may be used to estimate the concentration of K^+ in solution for the low water contents of the soil column.

4.8.2 Experimental verification of the reliability of the method of estimating concentration of K^+ in solution during horizontal infiltration

In order to verify the reliability of the method proposed in Section 4.8.1 for estimating the concentration of K^+ in solution during horizontal infiltration experiments, 5.0 g of Ca-saturated Brookston clay whose air-dry moisture content had previously been determined, were first equilibrated with 5 ml of 1.0M KCl solution in a 25 ml centrifuge tube for two hours. Eight replicate samples were used. After equilibration, three of the tubes were centrifuged and the supernatant solution analysed for K^+ using Atomic Absorption Spectrophotometer. The concentration of K^+ obtained from these three replicates served as the measured equilibrium concentration of K^+ in the initial equilibration which represents the equilibrium concentration in the horizontal infiltration experiment. At this stage the volume of liquid is the sum of the initial air-dry water content and the 5.0 ml of 1.0M KCl solution added.

Five milliliters of 0.5M KCl were then added to the contents of each of the remaining five centrifuge tubes and equilibrated again for two more hours on a reciprocating shaker, after which the tubes were centrifuged and the supernatant solution analysed for K^+. The concentration of K^+ in this second equilibration was used to estimate the concentration of the first equilibrium solution and compared with the measured concentration for this first equilibration.

SAMPLE CALCULATION

The calculation was done for the verification experiment described in Section 4.8.2 and is similar to that employed in estimating the concentration of K^+ in solution in the infiltration experiments.

Mass of soil solids = 4.565 g

Volume of water in air dry soil = 0.435 cm^3

Volume of 1.0M KCl added = 5.0 cm^3

Therefore volume of liquid in system at first equilibration = 5.435 cm^3

$$Sa_i = \frac{Ma_i}{4.565} \text{ meq/g}, \qquad Cs_i = \frac{Ms_i}{5.435 \times 10^{-3}} \text{ meq/l}$$

$$Sa_{ie} = \frac{Ma_{ie}}{4.565} \text{ meq/g}, \qquad Cs_{ie} = \frac{Ms_{ie}}{10.435 \times 10^{-3}} = 645.78 \text{ meq/l}$$

Ms_{ie} = 6.7387 meq

Ma_{ie} = 0.8229 meq

Me (measured) = 2.4616 meq

Therefore, from equation 4.7,

$$Ma_i + Ms_i = (6.7387 + 0.8229) - 2.4616$$
$$= 5.10 \text{ meq.}$$

From equation 4.9 we obtain the equation

$$5.10 = Ms_i + 4.565\left(10^{-0.1029\log^2\left(\frac{Ms_i}{5.435\times10^{-3}}\right) + 0.7444\log\left(\frac{Ms_i}{5.435\times10^{-3}}\right) - 2.0231}\right)$$

Ms_i = 4.2519

Cs_i = 782.32

Sa_i = 0.1858

The measured equilibrium concentration of K^+ and the concentration of K^+ calculated using the technique and theoretical procedure outlined above, are given in Table 4.2. It is observed that the agreement between measured and calculated concentration of K^+ in solution is good.

TABLE 4.2 Measured and computed concentration of K^+ in solution using the method proposed in the text (Brookston clay)

Replicate Number	Calculated Concentration (keq/m^3)	Measured Equilibrium Concentrations (keq/m^3)	% Error = $\frac{\text{(Calc-Measured)x100}}{\text{Measured}}$
1	-	0.7801	
2	-	0.7801	
3	-	0.7801	
4	0.7823		+0.3
5	0.7823		+0.3
6	0.7823		+0.3
7	0.7823		+0.3
8	0.7823		+0.3

4.8.3 Determination of concentration of Cl^- in solution during the infiltration experiment

Each of the oven dried subsamples from the determination of gravimetric water content of each section was shaken with 150 ml distilled water for 30 minutes on a reciprocating shaker. The extract was centrifuged and chloride in the clear supernatant solution determined using a method similar to the Technicon Auto Analyzer Industrial method no. 99-70W.

4.9 Computer programming method used to analyse data

The computation of the moisture diffusivity D, the dispersion coefficient D_s and subsequent simulation of (i) moisture content θ as a function of $\lambda(=x/\sqrt{t})$ and (ii) concentration of Cl^- or K^+ in solution c as a function of λ using the computed values of D and D_s were done with a computer program written in System 360 CSMP (I.B.M. 1972) whose statements also obey FORTRAN conventions.

Each program consists of three segments: INITIAL, DYNAMIC and TERMINAL. All operations specified in the INITIAL part of the program are carried out prior to the computation or simulation and are not repeated every time step. The operations in the DYNAMIC section, however, are performed repeatedly and updated for each elapsed time-interval during the period of simulation. Finally, the TERMINAL part consists of calculations or decisions which are to be made only after the dynamic procedure has been completed. It must be noted that segmenting a program is not mandatory in CSMP and that if a program is not segmented, the computer automatically assumes the entire program to be DYNAMIC. A concise description of CSMP is given in the User Manual (I.B.M. 1972). Detailed explanations of the principles and procedures of CSMP have been provided by Brennan and Silberberg (1968) and Speckhart and Green (1976). CSMP models for simulation of some soil physical processes have been published by Wierenga and de Wit (1970) and also Hillel (1977). Therefore, only the principal features of CSMP language which were found to be useful in this study will in general terms be discussed.

Perhaps the most powerful and important features of CSMP which make it particularly amenable to this study are the statements which cause (i) integration to be performed with time, and (ii) differentiation to be performed with respect to time. The general form of statements for these mathematical operations are:

$$Y = \text{INTGRL}(IC,X) \tag{4.10}$$

$$X = \text{DERIV}(IC,Y) \tag{4.11}$$

Equation 4.10 calculates the output variable Y by integrating the differential function X, with the initial condition that Y at the start of computation is equal to IC. Using a METHOD statement, a choice may be made among seven numerical integration techniques, two of which use the variable time step of integration whilst the others use a fixed time step of integration.

Equation 4.11, on the other hand, calculates the derivative output X by differentiating the integrated function Y with the initial condition that X at the start of computation is equal to IC.

Another feature of CSMP which was frequently used in this study is the calculation of definite integrals. Definite integrals were performed by instructing the computer to use the final time step value of the variable integration. This specification is put in the TERMINAL section. For an illustration of this feature, consider the calculation of equation 4.12, where t_f is the final time of integration.

$$\int_{t_f}^{t} Ydt = \int_{o}^{t} Ydt - \int_{o}^{t_f} Ydt \qquad (4.12)$$

The definite integral on the right hand side of equation 4.12, designated KON, may be evaluated by specifying to the computer to set KON=B where

B = INTGRL(IC,Y)

4.9.1 Description of the computer program for calculating the soil moisture diffusivity D(θ) and simulation of θ(λ) using the calculated D(θ) values

The actual program for Brookston clay written in System 360 CSMP is presented in fig. 4.5 (see also Appendix E for a similar program for Akuse soil). The governing equations are equations 3.11b and its solution (equation 3.13). Integration in CSMP is performed with respect to time. Renaming time equal to lambda, however, enables integration to be performed with respect to lambda. The integral $\int_{\theta_n}^{\theta} \lambda d\theta$ in equation 3.13 is rewritten so that integration is carried out with respect to λ instead of θ as follows:

FIGURE 4.5.

CSMP listing for calculating soil water diffusivity D as a function of water content θ and simulation of water content as a function of $\lambda(=xt^{-1/2})$ from the calculated D(θ) values for Brookston clay.

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                ****CONTINUOUS SYSTEM MODELING PROGRAM****

                          *** VERSION 1.3 ***

       TITLE CALCULATION OF SOIL MOISTURE DIFFUSIVITY AND SIMULATION OF
       TITLE WATER CONTENT AS A FUNCTION OF LAMBDA. (BROOKSTON CLAY)
       *     UNITS
       *     KG=KILOGRAMS
       *     M=METERS
       *     S=SECONDS
       *     GLOSSARY OF SYMBOLS
       *     DTHLAO=DERIVATIVE OF THE THETA-LAMBDA FUNCTION AT LAMBDA EQUALS
       *     ZERO
       *     THETAO=WATER CONTENT AT LAMBDA EQUALS ZERO
       *     LAMDAN=LAMBDA AT INFINITY (=FINTIM)
       *     THETAN=INITIAL WATER CONTENT
       *     THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
       *     RVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY AND THE DERIVATIVE
       *     OF THE THETA-LAMBDA FUNCTION
       *     RVELO=RVEL AT LAMBDA EQUALS ZERO
       *     D=SOIL WATER DIFFUSIVITY
       *     RDIV=DERIVATIVE OF RVEL WITH RESPECT TO LAMBDA
       *     RVELAO=RVELO MULTIPLIED BY 1.0001
       *     RVELA=HALF PAIR OF RVEL THROUGH THE FACTOR 1.0001 IN RVELAO
       *     RDIVA=HALF PAIR OF RDIV THROUGH THE FACTOR 1.0001
       *     THETA2=SIMULATED WATER CONTENT
       *     THETAA=HALF PAIR OF THETA2 THROUGH THE FACTOR 1.0001
       *     DRVEL=CORRECTION FACTOR
       *     DTHETA=DIFFERENCE BETWEEN THETA2 AND THETAA
       *     SLOPE=RATIO OF THE DIFFERENCE BETWEEN THETAA AND THETA2 TO THE
       *     DIFFERENCE BETWEEN RVELAO AND RVELO
       *     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
         RENAME TIME=LAMBDA
       INITIAL
              PARAMETER DTHLAO=-5.0,THETAO=.53,LAMDAN=1.82E-03,...
              THETAN=.12,KON2=1.0,RVELO=-.33[illegible]E-03,DEL=.0001,J=[illegible],I=[illegible]
              RVELAO=RVELO*(1.0+DEL)
              FUNCTION TBTHLA=(0.0,.53),(1.0E-04,.525),(3.0E-04,.52),...
              (5.0E-04,.515),(7.0E-04,.51),(9.0E-04,.50),(1.0E-03,.495),...
              (1.1E-03,.49),(1.2E-03,.48),(1.3E-03,.473),(1.4E-03,.463),...
              (1.5E-03,.445),(1.55E-03,.435),(1.6E-03,.42),(1.65E-03,.40),...
              (1.7E-03,.37),(1.75E-03,.325),(1.78E-03,.28),(1.8E-03,.235),...
              (1.81E-03,.185),(1.82E-03,.12),(1.9E-03,.12),(2.0E-03,.12)
       DYNAMIC
              THLA=NLFGEN(TBTHLA,LAMBDA)
              DTHLA=DERIV(DTHLAO,THLA)
              THETA1=INTGRL(THETAO,CTHLA)
              C=INTGRL(0.0,THLA)
              KON1=THETAN*LAMDAN
              E=(THLA*LAMBDA)-KON1
              FF=E-C
              G=FF+KON2
              D=-.5*G/DTHLA
              NOSORT
              IF(J.LE.2) GO TO 10
              SORT
              RVEL=INTGRL(RVELO,RDIV)
              RVELA=INTGRL(RVELAO,RDIVA)
              RDIV=-LAMBDA*RVEL*.5/D
              RDIVA=-LAMBDA*RVELA*.5/D
              THETA2=INTGRL(THETAO,RVEL/D)
              THETAA=INTGRL(THETAO,RVELA/D)
              NOSORT
          10  CONTINUE
```

```
      TERMINAL
             TIMER FINTIM=1.82E-03,PRDEL=3.60E-05
             PRINT G,THETAA.D,THETA1,THLA.THETA2
             IF(J.GE.3) GC TO 15
             J=J+1
             KON2=C
             GO TO 20
         15  I=I+1
             IF(ABS(THETA2-THETAN).LT..00001) STOP
             DTHETA=THETAA-THETA2
             SLOPE=DTHETA/DEL/RVELC
             DRVEL=(THETA2-THETAN)/SLOPE
             RVELO=RVELO-DRVEL
             RVELAO=RVELC*(1.0+DEL)
             WRITE(6,100) THETAA,D,THLA,THETA1,THETA2
        100  FORMAT(///' THETAA.D,THLA,THETA1.THETA2=',5E15.6)
             WRITE (6.101) RVELO.RVELAO
        101  FORMAT(//' CALL RERUN WITH RVELC,RVELAO=',2E20.7)
         20  IF(J.GT.10) STOP
             IF(I.GT.4) STOP
             CALL RERUN
      END
      STOP

OUTPUT VARIABLE SEQUENCE
RVELAO THLA   DTHLA  THETA1 C       KON1   E      EE     G      D
ZZ0004 RDIV   RVEL   RDIVA  RVELA  ZZ0008 THETA2 ZZ0010 THETAA ZZ0011
ZZ0012 J      KON2   I      DTHETA SLOPE  DRVEL  RVELO  RVELAO

 OUTPUTS    INPUTS   PARAMS  INTEGS + MEM BLKS  FORTRAN  DATA CDS
 33(500)  71(1400)  12(400)   6+  0=  6(300)   39(600)      13

      ENDJOB
```

Using integration by parts

$$u = \lambda \qquad dv = d\theta$$

$$du = d\lambda \qquad v = \theta$$

$$\int_{\theta_n}^{\theta} \lambda d\theta = uv \Big|_{\theta_n}^{\theta} - \int vdu$$

Therefore,

$$\int_{\theta}^{\theta} \lambda d\theta = \theta\lambda \Big|_{\theta_n}^{\theta} - \int_{\lambda_n}^{\lambda} \theta d\lambda$$

$$= \theta\lambda - \theta_n\lambda_n - \int_{\lambda_n}^{\lambda} \theta d\lambda \qquad (4.13)$$

Since integration by the computer necessarily always commences from time=0 (in this case $\lambda=0$), $\int_{\lambda_n}^{\lambda} \theta d\lambda$ was then rewritten such that integration would start from zero as follows:

$$\int_{0}^{\lambda_n=\infty} \theta d\lambda = \int_{0}^{\lambda} \theta d\lambda + \int_{\lambda}^{\lambda_n=\infty} \theta d\lambda \qquad (4.14)$$

$$\int_{\theta_n}^{\theta} \lambda d\theta = \theta\lambda - \theta_n\lambda_n + \int_0^{\lambda_n=\infty} \theta d\lambda - \int_0^{\lambda} \theta d\lambda \tag{4.15}$$

The governing equation 3.13 for the calculation of D therefore becomes

$$D = -\frac{1}{2}\frac{d\lambda}{d\theta}\left[\theta\lambda - \theta_n\lambda_n + \int_0^{\lambda_n=\infty} \theta d\lambda - \int_0^{\lambda} \theta d\lambda\right] \tag{4.16}$$

The D values obtained from equation 4.16 were then used to simulate $\theta(\lambda)$ by multiplying the second term of equation 3.11b by $\frac{D(\theta)}{D(\theta)}$ and rearranging it as follows:

$$\frac{d}{d\lambda}\left[D(\theta)\frac{d\theta}{d\lambda}\right] = -\frac{\lambda}{2}\frac{D(\theta)}{D(\theta)}\frac{d\theta}{d\lambda} \tag{4.17}$$

Letting $y = D(\theta)\frac{d\theta}{d\lambda} = \text{RVEL}$ (4.18)

equation 4.17 becomes

$$\text{RDIV} = \frac{dy}{d\lambda} = -\frac{\lambda y}{2D(\theta)} \tag{4.19}$$

The INITIAL section begins with specifiable constants DTHLAO, the derivative of the $\theta(\lambda)$ function at $\lambda=0$; THETAO, the moisture content at $\lambda=0$; LAMDAN, the final λ where the initial moisture content is THETAN; KON2 which is the definite integral $\int_0^{\lambda_n} \theta d\lambda$ but because it is not known at this stage, is set equal to 1.0 in the PARAMETER section. The actual value of KON2 is used after the first set of calculations through CALL RERUN and the specification KON2=C in the TERMINAL section. The counters J and I are initialised in the INITIAL section. Also the relation between RVELAO and RVELO is defined. It has to be mentioned that the multiplying factor may be made smaller, for example 1.00001, in which case the value of .0001 used for the slope must be changed to .00001 in the algorithm at the TERMINAL section. (Steps in the algorithm are given in Appendix C.) Function TBTHLA is a table of volumetric water content θ versus lambda (λ) read from a curve obtained from the horizontal infiltration experiment. In this table, the first values of each bracket are λ values (independent variables) and the second values are the corresponding moisture contents (dependent variables), arranged such that the independent variables are in a descending order of magnitude.

In the DYNAMIC section, the following calculations are made and updated at each time step during the simulation:

(1) Volumetric moisture content is read from the table of $\theta(\lambda)$ provided in FUNCTION TBTHLA through a Lagrange quadratic interpolation between points from:

THLA = NLFGEN(TBTHLA, LAMBDA) (4.20)

where NLFGEN designates the arbitrary non linear function generator of CSMP for tabular pairs of x, y coordinates.

(2) The derivative, $d\theta/d\lambda$ which is the rate of change of the volumetric water content with lambda:

DTHLA = DERIV(DTHLAO, THLA) (4.21)

(3) The derivatives of the $\theta(\lambda)$ function computed in equation 4.21 are integrated again, as a check on the differentiation procedure:

THETAI = INTGRL(THETAO,DTHLA) (4.22)

(4) The integral $\int_0^\lambda \theta d\lambda$ is evaluated:

C = INTGRL(0.0, THLA) (4.23)

(5) KON1 which is equal to the product of θ_n and λ_n is calculated and then $(\theta\lambda - \theta_n\lambda_n)$ evaluated:

KON1 = THETAN * LAMDAN (4.24a)

E = (THLA * LAMBDA) - KON1 (4.24b)

(6) $(\theta\lambda - \theta_n\lambda_n - \int_0^\lambda \theta d\lambda)$ is then calculated:

FF = E - C (4.25)

(7) The terms in brackets on the righthand side of equation 4.16 are calculated:

G = FF + KON2 (4.26)

where KON2, initially set equal to 1.0, is the definite integral $\int_0^{\lambda_n=\infty} \theta d\lambda$.

(8) The soil moisture diffusivity is then calculated by dividing the product of -.5 and G by the derivative $d\theta/d\lambda$(DTHLA):

D = -.5*G/DTHLA (4.27)

So far, the program only calculates $D(\theta)$ or $D(\lambda)$. There is then specification NOSORT which is necessary any time an IF statement is invoked or if the computer is required to perform operations in the sequence listed. The IF statement listed in fig. 4.5 requires that computation should bypass the statements immediately following the IF statement for the first two iterations. It is only when the counter $J \geq 3$ that simulation of $\theta(\lambda)$ is started. This stipulation is necessary because the value of the definite integral KON2 is known only when $J \geq 1$ and so the correct values of D for simulation are obtained when $J \geq 1$.

(9) Calculation of y (RVEL) by integrating, $dy/d\lambda$ (RDIV) (equation 4.19) is executed:

RVEL = INTGRL(RVELO,RDIV) (4.28)

RVELO is first estimated and specified in the PARAMETER section. Successive values of RVELO are calculated using the algorithm in the TERMINAL section, until either (a) the absolute value of the difference between the simulated moisture content at FINTIM and the initial moisture content is less than .00001, (b) J is greater than 10 or (c) counter I is greater than 6.

(10) Equation 4.19 is used to calculate $dy/d\lambda$ (RDIV)

RDIV = -LAMBDA * RVEL * .5/D (4.29)

(11) Simulated θ, designated THETA2, are obtained from the integration of equation 4.18:

THETA2 = INTGRL(THETAO, RVEL/D) (4.30)

As explained in Appendix C, equations 4.28, 4.29 and 4.30 are paired by multiplying the initial condition RVELO of equation 4.28, by a factor which in this example was 1.0001. Consequently we have

RVELA = INTGRL(RVELAO, RDIVA) (4.31)

RDIVA = -LAMBDA*RVELA*.5/D (4.32)

THETAA = INTGRL(THETAO, RVELA/D) (4.33)

The TERMINAL section includes statements of the total simulation time to be run (FINTIM), the time intervals for printing the output (PRDEL) and the list of output variables to be printed. This section also specifies that after the first iteration where J=0 and KON2=1.0, the value of KON2 in the second and subsequent iterations should be set equal to the last value obtained in the calculation of equation 4.23. In addition, this section contains the algorithm for the computation of RVELO, RVELAO and other iterations.

When there is no METHOD statement in the TERMINAL as with this program, the method of integration used is the Runge-Kutta fourth order variable time step procedure. Finally, the TERMINAL section has two WRITE statements. The first write statement specifies that values of 5 output variables in E-format* with a total of fifteen digits and a 6 decimal place should be printed for each iteration. The second write statement specifies that RVELO and RVELAO values used for each iteration should be printed.

4.9.2 Description of the computer program for calculating dispersion coefficient $D_s(\lambda)$ and simulation of $c(\lambda)$ using the calculated $D_s(\lambda)$ values

The computer program for calculating D_s for Cl^- and then simulating $c(\lambda)$ for Brookston clay, also written in system 360 CSMP, is given in fig. 4.6 and also Appendix F which is a similar program for Akuse clay. Many of the features in this program are similar to those of the preceding program. Enough of the features, however, are new to warrant a complete (albeit partially repetitive) explanation. The governing equations are equations 3.18b and 3.18c. Using equation 4.15, $g(\theta)$ in equations 3.18b and 3.18c is written as

$$g(\theta) = \theta\lambda - [\theta\lambda - \theta_n\lambda_n + \int_0^{\lambda=\infty} \theta d\lambda - \int_0^{\lambda} \theta d\lambda]$$

$$= \theta_n\lambda_n - \int_0^{\lambda_n=\infty} \theta d\lambda + \int_0^{\lambda} \theta d\lambda \qquad (4.34)$$

---

* For very large numbers or small numbers the format involving the letter E is used in CSMP, for example 1.7647E-14 is equivalent to 1.7647×10^{-14}.

FIGURE 4.6

CSMP listing for calculating dispersion coefficient D_s for Cl^- and simulation of $c(\lambda)$ from the computed $D_s(\lambda)$ values using (i) the analytical solution, and (ii) the computer solution described in the text.

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                               *** VERSION 1.3 ***

         TITLE DISPERSION COEFFICIENT AND SIMULATION OF CONC. (BROOKSTON CLAY)
         *     UNITS
         *     KEQ=KILO-EQUIVALENTS
         *     M=METERS
         *     S=SECONDS
         *     GLOSSARY OF SYMBOLS
         *     DTHLAO=DERIVATIVE OF THETA-LAMBDA FUNCTION AT LAMBDA
         *     EQUALS ZERO
         *     DTHLA=DERIVATIVE OF THETA -LAMBDA FUNCTION
         *     THETAO=VOLUMETRIC WATER CONTENT AT LAMBDA EQUALS ZERO
         *     LAMDAN=LAMBDA AT INFINITY (=FINTIM)
         *     THETAN=INITIAL WATER CONTENT
         *     THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
         *     VELC=THE PRODUCT OF WATER CONTENT, DISPERSION COEFFICIENT
         *     AND THE DERIVATIVE OF THE CONTRATION-LAMBDA FUNCTION
         *     VELCO=VELC AT LAMBDA EQUALS ZERO
         *     VELCAO=VELCO MULTIPLIED BY 1.00001
         *     SEEO=CONCENTRATION OF CHLORIDE IN SOLUTION AT LAMBDA EQUALS
         *     ZERO
         *     SEEN=INITIAL CONCENTRATION OF CHLORIDE IN MOIST SOIL
         *     DSEELA=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION WITH RESPECT
         *     TO LAMBDA
         *     DSELAO=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION AT LAMBDA
         *     EQUALS ZERO
         *     SEELA=INTERPOLATED CURVE FOR CONCENTRATION-LAMBDA FUNCTION
         *     LATHH=THE G-FUNCTION DEFINED IN EQUATION 4.34
         *     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
         *     TBSELA=TABLE OF CONCENTRATION OF CHLORIDE IN SOLUTION AND
         *     CORRESPONDING LAMBDA VALUES
         *     D=SOIL WATER DIFFUSIVITY
         *     DIV=DERIVATIVE OF VELC WITH RESPECT TO LAMBDA
         *     SEE2=SIMULATED CONCENTRATION OF CHLORIDE IN SOLUTION
         *     SEE1=CONCENTRATION OF CHLORIDE CALCULATED USING THE ANALYTICAL
         *     SOLUTION
         *     SEEA=HALF PAIR OF SEE2 THROUGH THE FACTOR 1.00001
         *     DVELC=CORRECTION FACTOR
         *     SLOPE=RATIO OF THE DIFFERENCE BETWEEN SEEA AND SEE2 TO THE
         *     DIFFERENCE BETWEEN VELCAO AND VELCO
         *     DSEE=DIFFERENCE BETWEEN SEE2 AND SEEA AT FINTIM
           RENAME TIME=LAMBDA
         INITIAL
                 INCON DSELAO=-1.0,SEEO=.97,SEEN=.005,VELCO=-.2678232E-04
                 PARAMETER DTHLAO=-5.0,THETAO=.53,LAMDAN=1.82E-03,J=0,I=0
                 CONSTANT THETAN=.12,KON2=1.0,KON3=1.0,KON4=1.0,DEL=.00001
                 VELCAO=VELCO*(1.0+DEL)
                 FUNCTION TBTHLA=(0.0,.53),(1.0E-04,.525),(3.0E-04,.52),...
                 (5.0E-04,.515),(7.0E-04,.51),(9.0E-04,.50),(1.0E-03,.495),...
                 (1.1E-03,.49),(1.2E-03,.48),(1.3E-03,.473),(1.4E-03,.463),...
                 (1.5E-03,.445),(1.55E-03,.435),(1.6E-03,.42),(1.65E-03,.4[illegible]),...
                 (1.7E-03,.37),(1.75E-03,.325),(1.78E-03,.28),(1.8E-03,.225),...
                 (1.81E-03,.185),(1.82E-03,.12),(1.9E-03,.12),(2.0E-03,.12)
                 FUNCTION TBSELA=(0.0,.97),(1.0E-04,.9699),(2.0E-04,.9698),...
                 (3.0E-04,.9697),(4.0E-04,.9696),(5.0E-04,.9695),...
                 (6.0E-04,.9694),(7.0E-04,.9693),(8.0E-04,.9692),...
                 (9.0E-04,.96),(1.0E-03,.95),(1.1E-03,.93),(1.2E-03,.895),...
                 (1.25E-03,.87),(1.3E-03,.825),(1.3[illegible]E-03,.76[illegible]),...
                 (1.4E-03,.64),(1.42E-03,.54),(1.43E-03,.49),(1.44E-03,.40),...
                 (1.45E-03,.35),(1.46E-03,.30),(1.47E-03,.25),(1.48E-03,.20),...
                 (1.49E-03,.18),(1.50E-03,.15),(1.52E-03,.12),(1.54E-03,.09),...
                 (1.55E-03,.085),(1.56E-03,.075),(1.57E-03,.065),...
```

```
              (1.58E-03,.06),(1.595E-03,.05),(1.615E-03,.04),...
              (1.63E-03,.03),(1.655E-03,.025),(1.67E-03,.02),(1.7E-3,.015)
              (1.75E-03,.01),(1.82E-03,.005),(1.9E-03,.001),(2.0E-3,0.0)
      DYNAMIC
              THLA=NLFGEN(TBTHLA,LAMBDA)
              SEELA=NLFGEN(TBSELA,LAMBDA)
              CTHETA=(THLA-THETAN)/(THETAO-THETAN)
              CSEE=(SEELA-SEEN)/(SEEO-SEEN)
              DTHLA=DERIV(DTHLAO,THLA)
              DSEELA=DERIV(DSELAO,SEELA)
              C=INTGRL(0.0,THLA)
              KON1=THETAN*LAMDAN
              E=(THLA*LAMBDA)-KON1
              FF=E-C
              G=FF+KON2
              D=-.5*G/DTHLA
              LATHH=(THLA*LAMBDA)+(2.0*D*DTHLA)
              GS=DSEELA*LATHH
              HS=INTGRL(0.0,GS)
              HS1=KON3-HS
              HS2=.5*HS1
              THDS=HS2/DSEELA
              DS=THDS/THLA
              NOSORT
              IF(I.LT.3) GO TO 10
              IF(THDS.EQ.0.0) GO TO 10
              SORT
              AH=LATHH/THDS
              BH=INTGRL(0.0,AH)
              CH=EXP(-.5*BH)
              MH=INTGRL(0.0,CH/THDS)
              RMH=MH/KON4
              SEE1=RMH*(SEEN-SEEO)+SEEO
              VELC=INTGRL(VELCO,RDIV)
              VELCA=INTGRL(VELCAO,RDIVA)
              RDIV=-(LATHH*VELC)/(2.0*THDS)
              RDIVA=-(LATHH*VELCA)/(2.0*THDS)
              SEE2=INTGRL(SEEO,VELC/THDS)
              SEEA=INTGRL(SEEO,VELCA/THDS)
              NOSORT
       10     CONTINUE
      TERMINAL
              METHOD SIMP
              PRINT THLA,D,THDS,DS,AH,SEELA,SEE1,SEE2
              TIMER FINTIM=1.82E-03,DELT=5.0E-06,PRDEL=3.64E-05
              I=I+1
              KON2=C
              KON3=HS
              IF(I.LT.4) GO TO 20
              KON4=MH
              IF(ABS(SEE2-SEEN).LT..000001) STOP
              DSEE=SEEA-SEE2
              SLOPE=DSEE/DEL/VELCO
              DVELC=(SEE2-SEEN)/SLOPE
              VELCO=VELCO-DVELC
              VELCAO=VELCO*(1.0+DEL)
              WRITE(6,100) KON2,KON3,KON4
      100     FORMAT(///' KON2,KON3,KON4=',3E15.6)
              WRITE(6,101) DSEE,SLOPE,DVELC
      101     FORMAT(///' DSEE,SLOPE,DVELC=',3E15.6)
              WRITE(6,103) VELCO,VELCAO
      103     FORMAT(//' CALL RERUN WITH VELCO,VELCAO=',2E20.7)
       20     IF(I.GT.10) STOP
              CALL RERUN
      END
      STOP
```

Designating $y = \theta D_s \frac{dc}{d\lambda}$ (4.35)

equation 3.18b becomes

$$\frac{dy}{d\lambda} = -\frac{g(\theta)}{2}\frac{dc}{d\lambda}$$

$$y\Big|_{y_n}^{y} = -\frac{1}{2}\int_{\lambda_n}^{\lambda} g(\theta)\frac{dc}{d\lambda}\,d\lambda \qquad (4.36)$$

y_n=0 because equations 3.20a and 3.20b imply that $\frac{dc}{d\lambda}$ at λ_n is zero. Also, because integration commences from time = 0, equation 4.36 was rewritten such that integration would start at λ=0 as follows:

$$y = \frac{1}{2}\left[\int_{0}^{\lambda_n=\infty} g(\theta)\frac{dc}{d\lambda}\,d\lambda - \int_{0}^{\lambda} g(\theta)\frac{dc}{d\lambda}\,d\lambda\right] \qquad (4.36)$$

Once y was obtained, θD_s and hence D_s were obtained by substitution into equation 4.35 to give

$$D_s = \frac{y}{\theta}\frac{d\lambda}{dc} \qquad (4.37)$$

Simulation of $c(\lambda)$ from the calculated D_s values is achieved by multiplying the second term on the lefthand side of equation 3.18b by $\theta D_s/\theta D_s$ and rearranging terms as follows:

$$\frac{d}{d\lambda}\left[\theta D_s\frac{dc}{d\lambda}\right] + \frac{g(\theta)}{2}\frac{\theta D_s}{\theta D_s}\frac{dc}{d\lambda} = 0 \qquad (4.38)$$

Substitution of equation 4.35 yields

$$\frac{dy}{d\lambda} = -\frac{g(\theta)}{2}\frac{y}{\theta D_s} \qquad (4.39)$$

Equations 4.39 and 4.35 are used in the algorithm to simulate c(λ). In addition, c(λ) data are also calculated using the analytical solution equation 3.21.

The first specification in the program is to rename time=lambda so that integration and differentiation would be performed with respect to lambda. The initial section then begins with constants specified in CSMP data statements INCON, PARAMETER and CONSTANT. These three data statements are completely equivalent and are used to assign numerical values. In figure 4.6, the following parameters or constants are assigned numerical values:

(1) DSELAO: derivative of c(λ) function at λ=0. This is estimated from the first two data points of the c(λ) curve which was used to provide data points for FUNCTION TBSELA.

(2) SEEO: concentration of chloride in solution at λ=0.

(3) SEEN: initial concentration of chloride in the dry soil before commencement of horizontal infiltration (i.e. concentration of chloride in solution at $\lambda=\lambda_n$ (LAMDAN).

(4) VELCO: first guess of the value of $\theta D_s \frac{dc}{d\lambda}$ at λ=0.

(5) DTHLAO: the derivative of θ(λ) at λ=0.

(6) THETAO: the volumetric water content at λ=0.

(7) THETAN: initial volumetric moisture content of soil before horizontal infiltration was started (i.e. moisture content at $\lambda=\lambda_n$).

(8) KON2: the definite integral $\int_0^{\lambda_n=\infty}\theta d\lambda$ in equation 4.34.

(9) KON3: the definite integral $\int_0^{\lambda_n=\infty} g(\theta)\frac{dc}{d\lambda}\, d\lambda$ in equation 4.36.

(10) KON4: the definite integral $M(\infty) = \int_0^{\lambda_n=\infty} [\frac{1}{\theta D_s} \exp(.5 \int_0^{\lambda} \frac{g}{\theta D_s}\, d\lambda)]\, d\lambda$ in equation 3.21.

As was done in the case of the simulation of $\theta(\lambda)$ using $D(\theta)$ values, KON2 and KON3 are initially assigned value of 1.0 but the actual values of KON2 and KON3 are used after the first iteration as specified in the TERMINAL section.

(11) The I and J counters are initialised.

Two tables are provided for $\theta(\lambda)$ and $c(\lambda)$ which respectively are labelled FUNCTION TBTHLA and FUNCTION TBSELA.

In the DYNAMIC section of the program, volumetric water content θ, and concentration of Cl^- in solution are respectively determined by quadratic interpolation of FUNCTION TBTHLA and FUNCTION TBSELA through the statements:

```
THLA  =  NLFGEN(TBTHLA, LAMBDA)                                  (4.40)
SEELA =  NLFGEN(TBSELA, LAMBDA)                                  (4.41)
```

The derivatives $d\theta/d\lambda$ and $dc/d\lambda$ are also performed respectively, using the statements:

```
DTHLA =  DERIV(DTHLAO, THLA)                                     (4.42)
DSEELA = DERIV(DSELAO, SEELA)                                    (4.43)
```

Equation 4.34 is then computed with the following statements:

```
C     = INTGRL(0.0, THLA)                              (4.44)
KON1  = THETAN*LAMDAN                                  (4.45)
B     = KON1+C                                         (4.46)
LATHH = B-KON2                                         (4.47)
```

Equations 4.44, 4.45, 4.46 and 4.47 compute respectively the terms $\int_0^{\lambda} \theta d\lambda$, $\theta_n \lambda_n$, $(\theta_n \lambda_n + \int_0^{\lambda} \theta d\lambda)$ and $g(\theta)$. KON2 of equation 4.47 is the definite integral $\int_0^{\lambda_n = \infty} \theta d\lambda$

Equation 4.36 is then solved by integrating the product of $g(\theta)$ and $dc/d\lambda$ as follows:

```
GS  =  DSEELA*LATHH                                    (4.48)
HS  =  INTGRL(0.0,GS)                                  (4.49)
HS1 =  KON3-HS                                         (4.50)
HS2 =  .5*HS1                                          (4.51)
```

The product $g(\theta) \frac{dc}{d\lambda}$ in equation 4.48 is integrated using the statement in equation 4.49. KON3 in equation 4.50 represents the definite integral $\int_0^{\lambda_n = \infty} g \frac{dc}{d\lambda} d\lambda$ and is assigned the value 1.0 for the first iteration. Like KON2, the correct magnitude of KON3 is used in subsequent iterations.

Having solved equation 4.36, θD_s and hence D_s are computed by the statements:

```
THDS  =  HS2/DSEELA                                          (4.52)
DS    =  THDS/THLA                                           (4.53)
```

Since the magnitude of KON2 and KON3 were for the first iteration assumed to be 1.0, more than one iteration is required to calculate the correct value of D_s. The IF statements in the program ensure that:

(1) at least three iterations are carried out before simulation is started, so that calculation of $c(\lambda)$ data is done with the correct D_s values, and

(2) avoid dividing by zero when calculating DIV, in case D_s is zero or $M(\infty)$ = KON4 is zero.

Concentration of Cl^- as a function of λ is first calculated using the analytical solution (equation 3.21). In this section of the program, the term $g(\theta)/\theta D_s$ is calculated using the statement:

```
AH = LATHH/THDS                                              (4.54a)
```

Equation 4.54a is then integrated and each integral value multiplied by -0.5 and exponentiated through the statements:

```
BH = INTGRL(0.0,AH)                                          (4.54b)
CH = EXP(-.5*BH)                                             (4.54c)
```

CH in equation 4.54c is divided by θD_s and integrated by the statement:

`MH = INTGRL(0.0,CH/THDS)` (4.54d)

The FINTIM value of MH is the value of the definite integral $M(\infty)$ in equation 3.21. MH is divided by $M(\infty)$ which is designated KON4 to obtain the righthand side of equation 3.21.

`RMH = MH/KON4` (4.54e)

Because the value of KON4 is not known initially, it is assigned the value of 1.0. The specification, KON4=MH in the TERMINAL section allows the FINTIM value calculated in equation 4.54d to be assigned to KON4. Concentration of Cl^- in solution as a function of λ is then calculated using the statement:

`SEEI = RMH*(SEEN-SEEO)+SEEO` (4.54f)

which is equivalent to

$$c = \frac{M(\lambda)}{M(\infty)} [c_n - c_o] + c_o \qquad (4.54g)$$

The simulation part of the program (figure 4.6) is similar to that of figure 4.5. y and $dy/d\lambda$ in equations 4.38 and 4.39 are designated VELC and DIV respectively. These are paired up through VELCO, the initial value of VELC so that

DIV = -(LATHH*VELC)/(2.0*THDS) (4.54h)

DIVA = -(LATHH*VELCA)/(2.0*THDS) (4.55)

VELC = INTGRL(VELCO,DIV) (4.56)

VELCA = INTGRL(VELCAO,DIVA) (4.57)

Equation 4.54.. is the CSMP version of equation 4.39. Integration of equation 4.39 which is done with the statement in equation 4.56 gives y (VELC). VELCA, whose initial value VELCAO= VELCO x 1.00001 is the half pair of VELC and it is used to generate the half pair of SEEO, namely SEEA and also DIVA (the half pair of DIV) through the algorithm in the TERMINAL section. Rearrangement of equation 4.38b and solving for c gives

$$c = c_o + \int_{\lambda=0}^{\lambda} y/\theta D_s \quad d\lambda$$

which is written in CSMP language as:

SEE2 = INTGRL(SEEO,VELC/THDS) (4.58a)

SEEA = INTGRL(SEEO,VELCA/THDS) (4.58b)

The TERMINAL section of figure 4.6 stipulates that Simpson's method of integration should be used to calculate all integrations. The total simulation time (FINTIM=$1.82\text{x}10^{-3}$), the time interval for printing the output PRDEL=$3.64\text{x}10^{-5}$ and the output variables to be printed are also specified. Statements instructing the computer to set the FINTIM value of computations in equations 4.44, 4.49 and 4.54d as KON2, KON3 and KON4 (i.e. the definite integrals $\int_0^{\lambda_n=\infty} \theta d\lambda$, $\int_0^{\lambda_n=\infty} g(\theta) \frac{dc}{d\lambda} d\lambda$ and $M(\infty)$) are also included in this section.

An algorithm (see details in Appendix D) similar to that for the simulation of $\theta(\lambda)$ in figure 4.5, which enables new values of VELCO and VELCAO to be calculated and used in subsequent iterations, is put under this TERMINAL section. Finally there are three WRITE statements, the format of two of which specifies that the FINTIM values of KON2, KON3, KON4, DSEE, SLOPE and DVEL be printed. The format of the third WRITE statement specifies that the new values of VELCO and VELCAO to be used in the next iteration should be printed. By examining these printed values of VELCO, a better estimate of VELCO than what was originally specified can be made if the first estimate does not converge quickly enough.

4.9.3 Description of the computer program for calculating dispersion coefficient $D_s(\lambda)$ for K^+ and simulation of $c(\lambda)$ using the calculated $D_s(\lambda)$ values

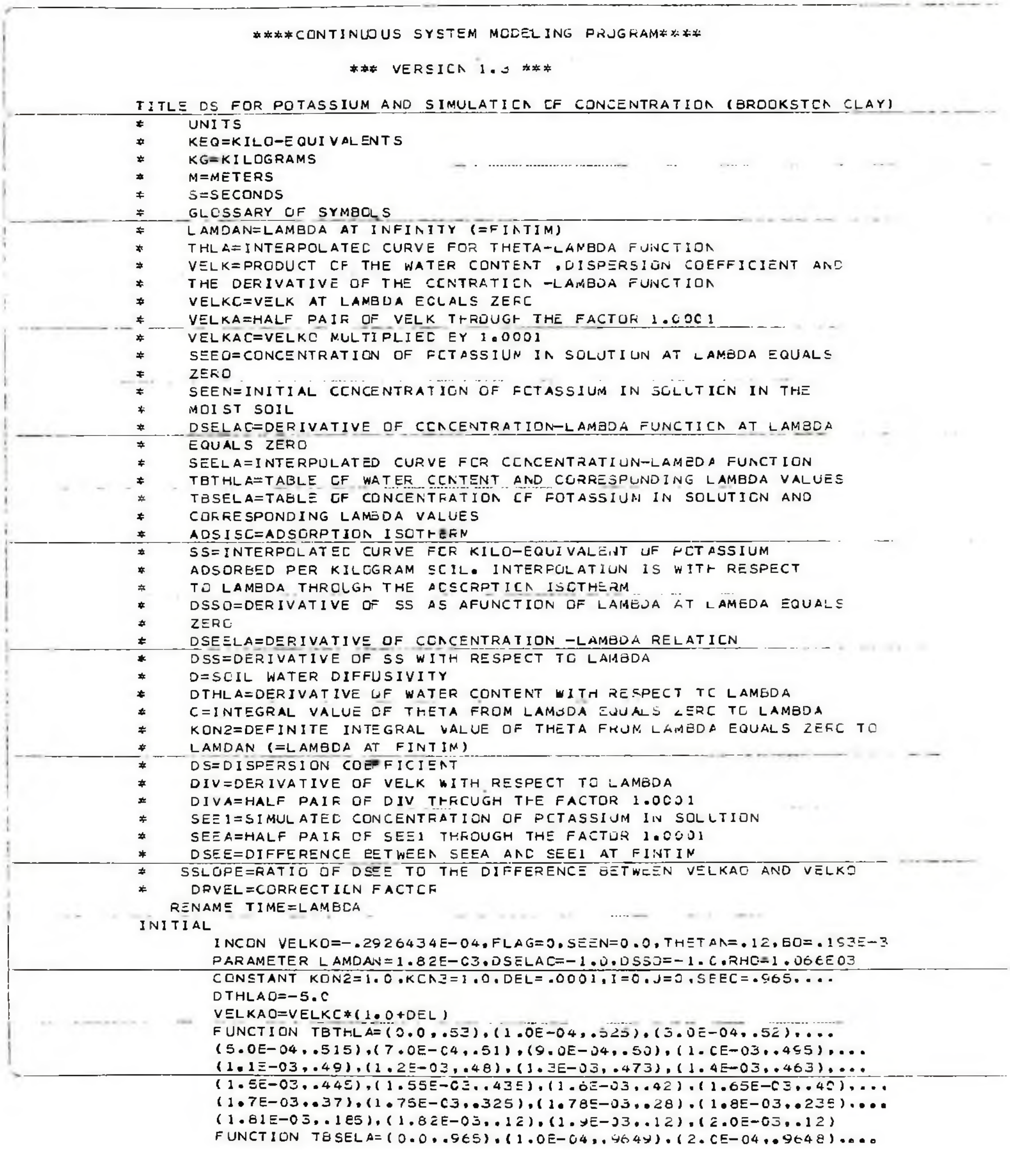
Like the other models used in this study, the calculation of $D_s(\lambda)$ for K^+ and the subsequent simulation of $c(\lambda)$ using the calculated $D_s(\lambda)$ values was programed in System 360 CSMP (Figure 4.7 and Appendix G). The governing equations are equations 3.19, 3.20a, 3.20b and 4.34.

$$\text{Letting } y = \theta D_s \frac{dc}{d\lambda} \tag{4.59}$$

equation 3.19 yields

FIGURE 4.7

CSMP listing for calculating dispersion coefficient D_s for K^+ and simulation of concentration of K^+ in solution as a function of $\lambda(=xt^{-1/2})$ for Brookston clay.



```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

TITLE DS FOR POTASSIUM AND SIMULATION OF CONCENTRATION (BROOKSTON CLAY)
*     UNITS
*     KEQ=KILO-EQUIVALENTS
*     KG=KILOGRAMS
*     M=METERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     LAMDAN=LAMBDA AT INFINITY (=FINTIM)
*     THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
*     VELK=PRODUCT OF THE WATER CONTENT ,DISPERSION COEFFICIENT AND
*     THE DERIVATIVE OF THE CENTRATION -LAMBDA FUNCTION
*     VELKO=VELK AT LAMBDA EQUALS ZERO
*     VELKA=HALF PAIR OF VELK THROUGH THE FACTOR 1.0001
*     VELKAO=VELKO MULTIPLIED BY 1.0001
*     SEEO=CONCENTRATION OF POTASSIUM IN SOLUTION AT LAMBDA EQUALS
*     ZERO
*     SEEN=INITIAL CONCENTRATION OF POTASSIUM IN SOLUTION IN THE
*     MOIST SOIL
*     DSELAO=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION AT LAMBDA
*     EQUALS ZERO
*     SEELA=INTERPOLATED CURVE FOR CONCENTRATION-LAMBDA FUNCTION
*     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
*     TBSELA=TABLE OF CONCENTRATION OF POTASSIUM IN SOLUTION AND
*     CORRESPONDING LAMBDA VALUES
*     ADSISO=ADSORPTION ISOTHERM
*     SS=INTERPOLATED CURVE FOR KILO-EQUIVALENT OF POTASSIUM
*     ADSORBED PER KILOGRAM SOIL. INTERPOLATION IS WITH RESPECT
*     TO LAMBDA THROUGH THE ADSORPTION ISOTHERM
*     DSSO=DERIVATIVE OF SS AS AFUNCTION OF LAMBDA AT LAMBDA EQUALS
*     ZERO
*     DSEELA=DERIVATIVE OF CONCENTRATION -LAMBDA RELATION
*     DSS=DERIVATIVE OF SS WITH RESPECT TO LAMBDA
*     D=SOIL WATER DIFFUSIVITY
*     DTHLA=DERIVATIVE OF WATER CONTENT WITH RESPECT TO LAMBDA
*     C=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO LAMBDA
*     KON2=DEFINITE INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO
*     LAMDAN (=LAMBDA AT FINTIM)
*     DS=DISPERSION COEFFICIENT
*     DIV=DERIVATIVE OF VELK WITH RESPECT TO LAMBDA
*     DIVA=HALF PAIR OF DIV THROUGH THE FACTOR 1.0001
*     SEE1=SIMULATED CONCENTRATION OF POTASSIUM IN SOLUTION
*     SEEA=HALF PAIR OF SEE1 THROUGH THE FACTOR 1.0001
*     DSEE=DIFFERENCE BETWEEN SEEA AND SEE1 AT FINTIM
*    SSLOPE=RATIO OF DSEE TO THE DIFFERENCE BETWEEN VELKAO AND VELKO
*     DRVEL=CORRECTION FACTOR
   RENAME TIME=LAMBDA
INITIAL
           INCON VELKO=-.2926434E-04,FLAG=0,SEEN=0.0,THETAN=.12,BO=.193E-3
           PARAMETER LAMDAN=1.82E-03,DSELAO=-1.0,DSSO=-1.0,RHO=1.066E03
           CONSTANT KON2=1.0,KON3=1.0,DEL=.0001,I=0,J=0,SEEO=.965,...
           DTHLAO=-5.0
           VELKAO=VELKO*(1.0+DEL)
           FUNCTION TBTHLA=(0.0,.53),(1.0E-04,.525),(3.0E-04,.52),...
           (5.0E-04,.515),(7.0E-04,.51),(9.0E-04,.50),(1.0E-03,.495),...
           (1.1E-03,.49),(1.2E-03,.48),(1.3E-03,.473),(1.4E-03,.463),...
           (1.5E-03,.445),(1.55E-03,.435),(1.6E-03,.42),(1.65E-03,.40),...
           (1.7E-03,.37),(1.75E-03,.325),(1.78E-03,.28),(1.8E-03,.235),...
           (1.81E-03,.185),(1.82E-03,.12),(1.9E-03,.12),(2.0E-03,.12)
           FUNCTION TBSELA=(0.0,.965),(1.0E-04,.9649),(2.0E-04,.9648),...
```

```
              (3.0E-04,.9647),(4.0E-04,.96),(5.0E-04,.955),(6.0E-04,.94),...
              (7.0E-04,.91),(8.0E-04,.85),(8.5E-04,.80),(9.0E-4,.70),...
              (9.3E-04,.60),(9.4E-04,.55),(9.5E-04,.47),(9.6E-04,.40),...
              (9.7E-04,.30),(9.8E-04,.24),(9.9E-04,.18),(1.0E-03,.14),...
              (1.01E-03,.125),(1.02E-03,.105),(1.03E-03,.09)...
              (1.04E-03,.075),(1.05E-03,.065),(1.06E-03,.055),...
              (1.07E-03,.045),(1.08E-03,.04),(1.09E-03,.035)...
              (1.1E-03,.03),(1.11E-03,.025),(1.12E-03,.023),...
              (1.13E-03,.02),(1.17E-03,.01),(1.2E-03,.006),...
              (1.21E-03,.0059),(1.219E-03,.00582),(1.2194E-03,.005816),...
              (1.22E-03,.0058),(1.23E-03,.0057)...
              (1.24E-03,.0056),(1.25E-03,.0055),(1.26E-03,.0054)...
              (1.27E-03,.0053),(1.28E-03,.0052),(1.29E-03,.0051)...
              (1.30E-03,.005),...
              (1.4E-03,.004),(1.5E-03,.003),(1.6E-03,.002),(1.7E-03,.001),...
              (1.82E-03,0.0),(2.0E-03,0.0)
              FUNCTION ADSISO=(1.0E-04,1.0E-06),(2.0E-04,2.5E-06)...
              (5.0E-04,5.6E-06),(1.0E-03,9.5E-06),(2.0E-03,1.55E-05),...
              (5.0E-03,2.8E-05),(.01,4.2E-05),(.021,6.0E-05),(.05,8.8E-05)...
              (.1,.115E-03),(.2,.143E-03),(.3,.155E-03),(.5,.175E-03),...
              (.7,.185E-03),(.9,.19E-03),(1.0,.195E-03)
       DYNAMIC
              THLA=NLFGEN(TBTHLA,LAMBDA)
              SEELA=NLFGEN(TBSELA,LAMBDA)
              SS=NLFGEN(ADSISO,SEELA)
              DTHLA=DERIV(DTHLAO,THLA)
              DSEELA=DERIV(DSELAO,SEELA)
              DSS=DERIV(DSSO,SS)
              AA=INTGRL(SEEO,DSEELA)
              C=INTGRL(0.0,THLA)
              BB=INTGRL(BO,DSS)
              KON1=THETAN*LAMDAN
              E=(THLA*LAMBDA)-KON1
              FF=E-C
              G=FF+KON2
              D=-.5*G/DTHLA
              E1=LAMBDA*RHO*DSS
              LATHAD=(.5*THLA*LAMBDA+D*DTHLA)*DSEELA+(.5*E1)
              G1=INTGRL(0.0,LATHAD)
              G2=KON3-G1
              THDS=G2/DSEELA
              DS=THDS/THLA
              NOSORT
              IF(FLAG.EQ.0.AND.I.LT.2) GO TO 10
              IF(THDS.EQ.0.0) GO TO 10
              SORT
              VELK=INTGRL(VELKO,DIV)
              VELKA=INTGRL(VELKAO,DIVA)
              DIV=(-.5*THLA*LAMBDA*VELK/THDS)-(D*VELK*DTHLA/THDS)-.5*E1
              DIVA=(-.5*THLA*LAMBDA*VELKA/THDS)-(D*VELKA*DTHLA/THDS)-.5*E1
              SEE1=INTGRL(SEEO,VELK/THDS)
              SEEA=INTGRL(SEEO,VELKA/THDS)
              NOSORT
         10   CONTINUE
       TERMINAL
              PRINT D,E,THLA,LATHAD,THDS,DS,SEELA,SEE1
              TIMER FINTIM=1.82E-03,PRDEL=3.64E-05,DELMIN=1.82E-20
              IF(FLAG.EQ.1) GO TO 15
              I=I+1
              KON2=C
              KON3=G1
              IF(I.GE.3) FLAG=1
              WRITE(6,100) KON2,KON3
        100   FORMAT(///' KON2,KON3=',2E15.6)
              IF(FLAG.EQ.0) GO TO 20
         15   J=J+1
```

```
                 IF(ABS(SEE1-SEEN).LT.1.0E-10) STOP
                 DSEE=SEEA-SEE1
                 SSLOPE=DSEE/DEL/VELKC
                 DRVEL=(SEE1-SEEN)/SSLCPE
                 VELKO=VELKO-DRVEL
                 VELKAO=VELKC*(1.0+DEL)
                 WRITE(6,101) DSEE,SSLCPE,DRVEL
            101  FORMAT(///' DSEE,SSLCPE,DRVEL=',3E15.6)
                 WRITE(6,102) VELKO,VELKAC
            102  FORMAT(//' CALL RERUN WITH VELKC,VELKAO=',2E20.7)
            20   IF(I.GT.10) STOP
                 IF(J.GT.7) STOP
                 CALL RERUN
           END
           STOP

OUTPUT VARIABLE SEQUENCE
VELKAO SEELA  DSEELA AA     THLA   C      SS     DSS    B8     E1
DTHLA  KON1   E      FF     G      D      LATHAD G1     G2     THDS
DS     ZZ0007 DIV    VELK   DIVA   VELKA  ZZ0011 SEE1   ZZ0013 SEEA
ZZ0014 ZZ0015 I      KON2   KON3   FLAG   J      DSEE   SSLOPE DRVEL
VELKC  VELKAO

 OUTPUTS     INPUTS    PARAMS  INTEGS + MEM BLKS  FORTRAN  DATA CDS
 46(500)  107(1400)  22(400)    8+  0=  8(300)  55(600)       36

           ENDJOB
```

$$\frac{dy}{d\lambda} = -\frac{1}{2}\left[g(\theta)\frac{dc}{d\lambda} + \lambda\rho\frac{dS}{d\lambda}\right], \qquad (4.60)$$

which upon integration and noting that equations 3.20a and 3.20b imply that $dc/d\lambda$ at λ_n is zero and therefore $y_n=0$, we obtain

$$y = -\frac{1}{2}\int_{\lambda_n}^{\lambda}\left[g(\theta)\frac{dc}{d\lambda} + \lambda\rho\frac{dS}{d\lambda}\right] d\lambda$$

$$\text{Let } B(\lambda) = g(\theta)\frac{dc}{d\lambda} + \lambda\rho\frac{dS}{d\lambda}$$

Therefore,

$$y = \frac{1}{2}\left[\int_0^{\lambda_n} B(\lambda)d\lambda - \int_0^{\lambda} B(\lambda)d\lambda\right] \qquad (4.61)$$

Substitution of equation 4.59 into 4.61 gives

$$\theta D_s = \frac{1}{2}\frac{d\lambda}{dc}\left[\int_0^{\lambda_n} B(\lambda)d\lambda - \int_0^{\lambda} B(\lambda)\, d\lambda\right] \qquad (4.62)$$

and

$$D_s = \theta D_s/\theta \qquad (4.63)$$

As with the case for the simulation of concentration of Cl^- in solution as a function of λ, the simulation of $c(\lambda)$ for K^+ was done by multiplying the second term of equation 3.19 by $\theta D_s/\theta D_s$ and substituting equation 4.59 to obtain

$$\frac{dy}{d\lambda} = - \frac{g(\theta)}{2} \frac{y}{\theta D_s} - \frac{\lambda\rho}{2} \frac{dS}{d\lambda} \tag{4.64}$$

Equations 4.59 and 4.64 are used in the algorithm to simulate $c(\lambda)$ for K^+.

Time was renamed lambda by the specification RENAME TIME=LAMBDA, so that integration and differentiation which are normally carried out with respect to time by the CSMP package would be performed in this case, with respect to lambda. The INITIAL section of this program also specifies constants such as VELKO ($=\theta D_s \frac{dc}{d\lambda}$ at $\lambda=0$); SEEN ($= c_n$ the initial concentration of K^+ in solution in the soil before commencement of horizontal infiltration with KCl solution); SEEO($= c_o$, the concentration of K^+ in solution at $\lambda=0$); THETAN ($=\theta_n$, the initial soil moisture content on volumetric basis); BO which is the keq. K^+ adsorbed per kg. soil at $\lambda=0$ and is estimated from the adsorption isotherm and concentration of K^+ in solution at $\lambda=0$; and LAMDAN($=\lambda_n$, the value of λ in the dry soil just adjacent to the wetting front. Other constants which are specified are:

(1) DSELAO: derivative of $c(\lambda)$ at $\lambda=0$ which is estimated from the first two data points of the $c(\lambda)$ curve used for FUNCTION TBSELA;

(2) DSSO: $dS/d\lambda$ at $\lambda=0$;

(3) RHO: the bulk density of the soil in the column;

(4) KON2: the definite integral $\int_0^{\lambda_n} \theta d\lambda$

(5) KON3: the definite integral $\int_0^{\lambda_n} B(\lambda) d\lambda$ in equation 4.61.

For the first iteration when I=0, KON2 and KON3 are not known and so are assigned arbitrary value of 1.0. Subsequent iterations, however, use the actual values of KON2 and KON3 because of the statement in the TERMINAL section setting KON2 and KON3 equal to the FINTIM value of their respective variable time step integrals.

The counters I and J are initialised and the relationship between VELKAO and VELKO through the multiplicative factor 1.0001 is also defined followed by tables TBTHLA, TBSELA and ADSISO which are experimental data points for $\theta(\lambda)$,$c(\lambda)$ and $SS(c)$ respectively.

In the DYNAMIC section, quadratic interpolation of TBTHLA, TBSELA and ADSISO provides values of volumetric moisture content, concentration of K^+ in solution, and amount of K^+ adsorbed for each lambda step, respectively, through the statements:

```
    THLA   = NLFGEN(TBTHLA, LAMBDA)                         (4.65)
   SEELA   = NLFGEN(TBSELA, LAMBDA)                         (4.66)
      SS   = NLFGEN(ADSISO, SEELA)                          (4.67)
```

Equation 4.67 provides $SS(\lambda)$ through the adsorption isotherm and $c(\lambda)$ interpolation.

The derivatives $dc/d\lambda$ and $dS/d\lambda$ are calculated respectively through the statements:

```
    DSEELA = DERIV(DSELAO, SEELA)                           (4.68)
    DSS    = DERIV(DSSO, SS)                                (4.69)
```

Equations 4.68 and 4.69 are integrated to serve as a check on the accuracy of the calculation of $dc/d\lambda$ and $dS/d\lambda$, through the statements:

```
    AA     = INTGRL(SEEO, DSEELA)                           (4.70)
```

```
BB    = INTGRL(BO, DSS)                                    (4.71)
```

The soil water diffusivity, D, is then calculated with statements similar to those in figure 4.5.

```
C     = INTGRL (0.0, THLA)                                 (4.72a)
KON1  = THETAN*LAMDAN                                      (4.72b)
E     = (THLA*LAMBDA)-KON1                                 (4.73a)
FF    = E-C                                                (4.73b)
G     = FF+KON2                                            (4.74a)
D     = -.5*G/DTHLA                                        (4.74b)
```

The second term $\lambda\rho dS/d\lambda$ of equation 4.60 and then equation 4.61 are calculated with the statements:

```
E1    = LAMBDA*RHO*DSS                                     (4.75)
LATHAD= (.5*THLA*LAMBDA+D*DTHLA)*DSEELA+(.5*E1)            (4.76)
G1    = INTGRL(0.0, LATHAD)                                (4.77)
G2    = KON3-G1                                            (4.78)
```

In equation 4.76, $(\theta\lambda + 2Dd\theta/d\lambda)$ which is equal to $g(\lambda)$ in equation 4.60 has been substituted so that in mathematical form we have

$$\text{LATHAD} = \frac{g}{2}\frac{dc}{d\lambda} + \frac{\lambda\rho}{2}\frac{ds}{d\lambda}$$

$$= \left(\frac{\theta\lambda}{2} + D\frac{d\theta}{d\lambda}\right)\frac{dc}{d\lambda} + \frac{\lambda\rho}{2}\frac{dS}{d\lambda}$$

θD_s and D_s are calculated with the statements:

```
THDS = G2/DSEELA                                              (4.79a)

DS   = THDS/THLA                                              (4.79b)
```

Simulation of $c(\lambda)$ follows when FLAG=1 after three iterations to obtain D, θD_s and D_s. Statements following the NOSORT specification (figure 4.7) ensure that three iterations are performed and also avoids division by zero if θD_s is zero. In order to simulate the $c(\lambda)$ for K^+, $(\theta\lambda + 2Dd\theta/d\lambda)$ is substituted for g and $dy/d\lambda$ is designated DIV in equation 4.64. Thus equation 4.64 becomes

$$\text{DIV} = -\frac{\theta\lambda\, y}{2\theta D_s} - D\frac{d\theta}{d\lambda}\frac{y}{\theta D_s} - \frac{\lambda\rho}{2}\frac{dS}{d\lambda} \qquad (4.80)$$

Integration of DIV with respect to λ then gives y which is designated VELK. In CSMP, equation 4.80 and its subsequent integration are calculated using the statements:

```
DIV = (-.5*THLA*LAMBDA*VELK/THDS) - (D*VELK*DTHLA/THDS)

         - .5*E1                                              (4.81)

VELK = INTGRL(VELKO, DIV)                                     (4.82)
```

The concentration of K^+ as a function of λ is obtained by integrating equation 4.59, that is:

$$\int_{c_0}^{c} dc = \int_{\lambda=0}^{\lambda} y/\theta D_s \, d\lambda$$

$$c = c_0 + \int_{\lambda=0}^{\lambda} y/\theta D_s \, d\lambda \tag{4.83}$$

Equation 4.83 is calculated with the statement:

```
SEE1 = INTGRL(SEEO, VELK/THDS)                                   (4.84)
```

As was done with the preceding simulations in this study, equations 4.81, 4.82 and 4.84 were paired through the factor 1.0001 of VELKO as follows:

```
VELKA = INTGRL(VELKAO, DIVA)                                     (4.85)
DIVA  = (-.5*THLA*LAMBDA*VELKA/THDS)-(D*VELKA*DTHLA/THDS)
        -.5*E1                                                   (4.86)
SEEA  = INTGRL(SEEO,VELKA/THDS)                                  (4.87)
```

In the TERMINAL section of figure 4.7, the total simulation time (FINTIM=$1.82\text{x}10^{-3}$), the time interval for printing the output, the minimum integration step DELMIN=1.82E-20, and the output variables to be printed, are specified. An IF statement specifies to the computer to start using the algorithm for simulation after three iterations when FLAG is set equal to 1. The algorithm for simulating $c(\lambda)$ for K^+ is similar to that employed in the simulation of $c(\lambda)$ for Cl^- (see Appendix D for details). Simulation stops if the difference between the simulated concentration at FINTIM and c_n is less than $1.0\text{x}10^{-10}$. If this convergence is not obtained after either ten iterations on the I counter or seven iterations on the J counter, simulation is then terminated. Examination of the WRITE output for VELKO and VELKAO then enables a better guess of VELKO which will ensure rapid convergence.

4.9.4 Description of the computer program for calculating the dispersion coefficient D_s for chloride in the case where anion exclusion occurs

The governing equations are 3.54, 3.55 and 3.58. It must be pointed out that $d\pi/d\lambda$ in equation 3.54 is the total osmotic pressure gradient. Its conversion to $dc/d\lambda$ using Van't Hoffs Law may over-estimate the effect of osmosis in the experiments considered in this study. This over-estimation was actually observed in our experiments because preliminary calculations indicated that the osmosis term on the righthand side of equation 3.54 dominated all other terms. Because the total osmotic pressure gradient is not known in our experiments, equation 3.54 was approximated by multiplying the second term in brackets on the righthand side by a factor β defined as:

$$\beta = \frac{c - c_{\text{expected}}}{c}$$

The assumption is made in the formulation of β that in the wet zone where the moisture content is near saturation, compensation between ions occurs so that osmotic pressure in this region may be very small or negligible.

In the horizontal infiltration experiment in this study, it was observed that the concentration distribution of K^+ was for all practical purposes zero at $\lambda = 1.2\text{x}10^{-3}$ $\text{ms}^{-1/2}$ and so the chloride present between $\lambda = 1.2\text{x}10^{-3}$ and $1.82\text{x}10^{-3}$ $\text{ms}^{-1/2}$ (the wetting front) is presumably linked with Ca^{2+} (see figure 5.9). Therefore, $d\pi/d\lambda$ in equation 3.54 was converted to c by using Van't Hoff's equation so that we have

$$d\pi/d\lambda \quad = \quad n\ RT\ dc/d\lambda$$

with n = 3/2 and c is the chloride concentration in keq. Cl^{-}/m^{3}.

Equation 3.54 therefore becomes:

$$-\frac{\theta\lambda}{2}\frac{dc}{d\lambda} + \frac{\lambda\theta_{ex}}{2}\frac{dc}{d\lambda} = \frac{d}{d\lambda}\left[(\theta D_s - \frac{3RT\sigma cK(\theta)}{2g\rho_w}\beta)\frac{dc}{d\lambda}\right] + D(\theta)\frac{d\theta}{d\lambda}\frac{dc}{d\lambda} - \frac{d}{d\lambda}(\sigma c D(\theta)\frac{d\theta}{d\lambda}) \qquad (4.88a)$$

Designating $(\theta D_s - \frac{3RT\sigma cK(\theta)}{g\rho_w}\beta)\frac{dc}{d\lambda} = y$ in equation 4.88a we have

$$\frac{dy}{d\lambda} = -\frac{\theta\lambda}{2}\frac{dc}{d\lambda} + \frac{\lambda\theta_{ex}}{2}\frac{dc}{d\lambda} - D(\theta)\frac{d\theta}{d\lambda}\frac{dc}{d\lambda} + \frac{d}{d\lambda}(\sigma c D(\theta)\frac{d\theta}{d\lambda})$$

which when integrated with the initial and boundary conditions formulated in equations 3.20a and 3.20b gives:

$$y = \int_{\lambda_n}^{\lambda}\left[\frac{\theta\lambda}{2}\frac{dc}{d\lambda} - \frac{\lambda\theta_{ex}}{2}\frac{dc}{d\lambda} + D(\theta)\frac{d\theta}{d\lambda}\frac{dc}{d\lambda} - \frac{d}{d\lambda}(\sigma c D(\theta)\frac{d\theta}{d\lambda})\right] d\lambda$$

$$= \int_{\lambda}^{\lambda}(H1 - H12 + H2 - H3)\ d\lambda \qquad (4.88b)$$

where

$$H1 = \frac{\theta\lambda}{2}\frac{dc}{d\lambda}$$

$$H12 = \frac{\lambda\theta_{ex}}{2} \frac{dc}{d\lambda}$$

$$H2 = D(\theta) \frac{d\theta}{d\lambda} \frac{dc}{d\lambda}$$

$$H3 = \frac{d}{d\lambda} (\sigma c D(\theta) \frac{d\theta}{d\lambda})$$

In order for integration to be started at $\lambda=0$, equation 4.88b was written as:

$$y = \int_0^{\lambda} {}^{\infty} P d\lambda - \int_0^{\lambda} P d\lambda \qquad (4.89)$$

where $P = H1 - H12 + H2 - H3$

Once y was calculated, θD_s and hence D_s was computed with equations 4.90a and 4.90b:

$$\theta D_s = (y \frac{d\lambda}{dc} + \frac{3RT\sigma cK(\theta)}{2g\rho_w} \beta) \qquad (4.90a)$$

$$D_s = \theta Ds/\theta \qquad (4.90b)$$

The actual computer program, also written in system 360 CSMP is given in figure 4.8. The units used in this program is the cg.s system and concentration is in moles per cm^3 because it is convenient to use the gas constant R in cg.s units. Time was first renamed lambda. The INITIAL section of the program then consists of specifiable constants provided in CSMP data statement. In figure 4.8, the following are assigned numerical values under data statements INCON, PARAMETER, or

FIGURE 4.8

CSMP listing for calculating dispersion coefficient D_s for Cl^- in the case where anion exclusion occurs (Akuse clay).

```
                ****CONTINUOUS SYSTEM MODELING PROGRAM****

                         *** VERSION 1.3 ***

*     DISPERSION COEFFICIENT WITH SALT SIEVING TERM IN EQUATION
*     UNITS
*     MOL=MOLES
*     G=GRAMS
*     CM=CENTIMETERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     SEEO=CONCENTRATION OF CHLORIDE IN THE INFILTRATING SOLUTION
*     R=UNIVERSAL GAS CONSTANT
*     T=TEMPERATURE
*     MRCO=DERIVATIVE OF MATRIC POTENTIAL WITH RESPECT TO LAMBDA
*     AH3=THE PRODUCT OF SIGMA,SOIL WATER DIFFUSIVITY ,CHLORIDE
*     CONCENTRATION AND THE DERIVATIVE OF WATER CONTENT WITH
*     RESPECT TO LAMBDA
*     HO3=THE DERIVATIVE OF AH3 WITH RESPECT TO LAMBDA
*     SEEN=INITIAL SOIL WATER CONTENT
*     THLAO=THE DERIVATIVE OF SOIL WATER CONTENT WITH RESPECT TO
*     LAMBDA EVALUATED AT LAMBDA EQUALS ZERO
*     MOLO=THE DERIVATIVE OF THE CONCENTRATION OF CHLORIDE IN MOLES
*     WITH RESPECT TO LAMBDA MEASURED AT LAMBDA EQUALS ZERO
*     THETAN=INITIAL WATER CONTENT OF SOIL
*     KON2=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO
*     LAMDAN (=LAMBDA AT FINTIM)
*     ACC=ACCELERATION DUE TO GRAVITY
*     RHOW=DENSITY OF WATER
*     KON4=THE DEFINITE INTEGRAL VALUE OF P FROM LAMBDA EQUALS ZERO
*     TO LAMDAN (=LAMBDA AT FINTIM) (EQUATION 4.89)
*     MSEEO=MEASURED CHLORIDE CONCENTRATION AT LAMBDA EQUALS ZERO
*     THETAO=SOIL WATER CONTENT AT LAMBDA EQUALS ZERO
*     SIGMA=THE REFLECTION COEFFICIENT
*     THETA=TABLE OF SOIL WATER CONTENT VERSUS LAMBDA
*     SEE=TABLE OF CHLORIDE CONCENTRATION IN SOLUTION AND
*     CORRESPONDING LAMBDA VALUES
*     MPOT=TABLE OF MATRIC POTENTIAL AND CORRESPONDING WATER CONTENT
*     VALUES
*     SEEXP=TABLE OF EXPECTED CHLORIDE CONCENTRATION VERSUS LAMBDA
*     MRC=WATER RETENTION CURVE
*     DMRC=DERIVATIVE OF THE WATER RETENTION CURVE WITH RESPECT TO
*     LAMBDA
*     THETEX=WATER CONTENT OF THE EXCLUSION ZONE
*     MOLES=CONCENTRATION OF CHLORIDE IN SOLUTION
*     SEELA=CONCENTRATION OF CHLORIDE IN MILLI-EQUIVALENT PER
*     CUBIC CENTIMETERS OF SOLUTION
   RENAME TIME=LAMDA
INITIAL
        INCON SEEO=1.0E-03,R=8.31432E07,T=296.0,MRCO=4.6374E02
        PARAMETER HO3=-2.6923E-06,SEEN=.01E-03,THLAO=-1.0,MOLO=-1.0E-04
        CONSTANT KON2=1.0,KON4=1.0,KON5=1.0E-03,THETAN=.05,...
        LAMDAN=1.82E-01,MSEEO=.91E-03,THETAO=.495,RHOW=1.0,ACC=980.6
        FUNCTION THETA=(0.0,.495),(5.0E-03,.49),(1.0E-02,.4875),...
        (2.0E-02,.485),(3.0E-02,.483),(4.0E-02,.48),(6.0E-02,.475),...
        (8.0E-02,.47),(1.0E-01,.465),(.11,.46),(.12,.455),...
        (.13,.445),(.136,.44),(.14,.435),(.15,.42),...
        (.155,.405),(.16,.39),(.165,.3675),...
        (.17,.3375),(.175,.29),(.18,.19),...
        (.182,.05),(.19,.05)
        FUNCTION SEE=(0.0,.93),(.01,.929),(.02,.928),(.03,.926),...
        (.04,.924),(.05,.922),(.06,.92),(.07,.91),(.08,.895),...
        (.085,.89),(.09,.875),(.095,.865),(.1,.85),(.105,.84),...
        (.11,.82),(.12,.81),(.13,.82),(.14,.83),...
```

```
          (.15,.845),(.155,.865),(.16,.90),(.165,.95),...
          (.17,1.01),(.175,1.14),(.176,1.2),(.182,.01)
          FUNCTION SEEXP=(0.C,.93),(.01,.929),(.02,.928),(.C3,.926),...
          (.04,.924),(.05,.922),(.06,.92),(.07,.91),(.08,.895),...
          (.085,.89),(.09,.875),(.095,.865),(.1,.85),(.105,.84),...
          (.11,.82),(.12,.8),(.13,.79),(.14,.78),(.15,.77),(.16,.76),...
          (.17,.755),(.176,.75),(.182,.01)
          FUNCTION MPOT=(.28,120.0),(.285,115.0),(.293,110.0),...
          (.2975,105.0),(.305,100.0),(.31,95.0),(.3175,90.0),...
          (.325,85.0),(.335,80.0),(.343,75.0),(.353,70.0),...
          (.363,65.0),(.375,60.C),(.3875,55.0),(.403,50.C),...
          (.4175,45.0),(.435,40.0),(.45,35.0),(.465,30.0),...
          (.483,25.0),(.495,20.0),(.51,15.0),(.5175,10.C),...
          (.525,5.0),(.53,0.0)
DYNAMIC
          THLA=AFGEN(THETA,LAMDA)
          SEELA=AFGEN(SEE,LAMDA)
          MRC=NLFGEN(MPOT,THLA)
          SEEXPT=AFGEN(SEEXP,LAMDA)
          A=DERIV(THLAC,THLA)
          DC=DERIV(MRCO,MRC)
          DMRC=-DC/A
          C=INTGRL(0.0,THLA)
          KON1=THETAN*LAMDAN
          E=(THLA*LAMDA)-KON1
          FF=E-C
          G=FF+KON2
          D=-.5*G/A
          HCOND=D/DMRC
          NOSORT
          IF(I.LE.3) GC TO 5
          SORT
          MOLES=KON5*SEELA
          C1=DERIV(MOLO,MOLES)
          SIGMAO=1.0-MSEED/SEEC
          THETEX=THETAC*SIGMAO
          SIGMA=THETEX/THLA
          BETA=(SEELA-SEEXPT)/SEELA
          AH3=SIGMA*MOLES*D*A
          H1=.5*THLA*LAMDA*C1
          H12=.5*THETEX*LAMDA*C1
          H2=D*A*C1
          H3=DERIV(HO3,AH3)
          H4=H1-H12+H2-H3
          H5=INTGRL(0.0,H4)
          Y=KON4-H5
          H7=Y/C1
          H8=(1.5*R*T*MOLES*SIGMA*HCOND*BETA)/(ACC*RHOW)
          THDS=H7+H8
          DS=THDS/THLA
          NOSORT
  5       CONTINUE
TERMINAL
          METHOD SIMP
          PRINT THLA,BETA,SEEXPT,H2,Y,H7,H8,DS
          TIMER FINTIM=1.82E-01,PRDEL=3.64E-03,DELT=1.1375E-04
          I=I+1
          KON2=C
          IF(I.LE.4) GC TO 20
          J=J+1
          KON4=H5
          WRITE(6,100) KON2,KON4
  100     FORMAT(///' KON2,KON4=',2E15.6)
  20      IF(I.GT.6) STOP
          IF(J.GT.4) STOP
          CALL RERUN
END
STOP
```

CONSTANT:

1. SEEO: concentration of Cl^- in moles per cm^3 in the infiltrating solution
2. R : gas constant in g/moles.K
3. T : temperature K
4. MRCO: $dH/d\lambda$ at $\lambda=0$ and H is the matric potential from the moisture retention curve provided as a table in FUNCTION MPOT
5. AH3: the product of σ, c, D and the derivative $d\theta/d\lambda$ of the $\theta(\lambda)$ curve given as a table in FUNCTION THETA
6. SEEN: initial concentration of chloride in the air dry soil
8. THLAO: $d\theta/d\lambda$ at $\lambda=0$
9. MOLO: $dc/d\lambda$ at $\lambda=0$ (c in $moles/cm^3$)
10. THETAN: initial moisture content
11. KON2: the definite integral $\int_0^{\lambda} \theta d\lambda$
12. ACC: acceleration due to gravity
13. RHOW: density of water
14. KON4: the definite integral $\int_0^{\lambda_n} P d\lambda$ in equation 4.89
15. KON5: factor to convert concentration in meq/cm^3 to $moles/cm^3$
16. LAMDAN: λ at FINTIM
17. MSEEO: measured concentration at $\lambda=0$.

Tables THETA, SEE, and MPOT which are experimental data points for $\theta(\lambda)$, $c(\lambda)$, and $H(\theta)$ respectively, are provided. Table for $c_{expected}$

as a function of λ, obtained by extrapolation of the linear portion of the experimental $c(\lambda)$ curve is given in FUNCTION SEEXP.

In the DYNAMIC section linear interpolation of Tables THETA, SEE, SEEXP and quadratic interpolation of Table MPOT provide values of volumetric water content, concentration in solution and expected c for each lambda step respectively, through the statements:

THLA = AFGEN(THETA, LAMBDA) (4.91)

SEELA = AFGEN(SEE, LAMBDA) (4.92)

SEEXPT = AFGEN(SEEXP, LAMBDA) (4.93)

MRC = NLFGEN(MPOT, THLA) (4.94)

The derivatives $d\theta/d\lambda$, $dH/d\lambda$ and $dh/d\theta$ are computed respectively through the statements:

A = DERIV(THLAO, THLA) (4.95)

DC = DERIV(MRCO, MRC) (4.96)

DMRC = -DC/A (4.97)

Then moisture diffusivity D is calculated (see description in sections 4.9.1, 4.9.2 and 4.9.3). Hydraulic conductivity is then computed by dividing D by $dH/d\theta$:

HCOND = D/DMRC (4.98)

An IF statement following equation 4.98 allows at least three iterations to be carried out so that the correct values of the moisture diffusivity are obtained since the correct value of KON2 is only known after the first iteration when KON2 is set equal to the last value of C in figure 4.8. Concentrations measured in meq/cm^3 are then converted into moles/cm^3 and the derivatives of the resulting $c(\lambda)$ curve computed with the following statements:

MOLES = KON5*SEELA (4.99)

C1 = DERIV(MOLO, MOLES) (4.100)

σ at $\lambda=0$ is computed from equation 3.55, then θ_{ex} is computed using the calculated σ at $\lambda=0$, after which equation 3.58 is used to calculate $\sigma(\lambda)$. The following statements are used to calculate σ at $\lambda=0$, θ_{ex}, and $\sigma(\lambda)$, respectively:

SIGMAO = 1.0-MSEEO/SEEO (4.101)

THETEX = THETAO*SIGMAO (4.102)

SIGMA = THETEX/THLA (4.103)

The correction factor β defined by equation 3.60a and the last term in brackets on the righthand side of equation 3.60b (viz: $\sigma c\ D(\theta)d\theta/d\lambda$) are computed through the statements:

BETA = (SEELA-SEEXPT)/SEELA (4.104)

AH3 = SIGMA*MOLES*D*A (4.105)

H1, H12, H2 and H3 in equation 4.88b are computed using the following statements:

```
H1  =  .5*THLA* LAMBDA*C1                                   (4.106)
H12 =  .5*THETEX*LAMBDA*C1                                  (4.107)
H2  =  D*A*C1                                               (4.108)
H3  = DERIV(HO3,AH3)                                        (4.109a)
H4  =  H1-H12+H2-H3                                         (4.109b)
```

H4 is then integrated with respect to λ and y (in equation 4.88) computed with the statements:

```
H5  =  INTGRL(0.0, H4)                                      (4.110)
Y   =  KON4-H5                                              (4.111)
```

KON4 is the definite integral $\int_0^{\lambda_n} P d\lambda$ in equation 4.89. For the first iteration its value is not known and so it is given a value of 1.0 specified in the PARAMETER statement. For subsequent iterations, the correct value of KON4 is used through the statement specified in the TERMINAL section that KON4 should be set equal to H5. The first and second terms in the brackets on the righthand side of equation 4.90a are computed through the statements:

```
H7  =  Y/C1                                                 (4.112)
H8  =  (1.5*R*T*MOLES*SIGMA*HCOND*BETA)/(ACC*RHOW)          (4.113)
```

Lastly, θD_s and D_s are calculated with the statements:

THDS = H7+H8 (4.114)

DS = THDS/THLA (4.115)

The TERMINAL section of figure 4.8 specifies that Simpson's integration method should be used for all integration procedures. The total simulation time (FINTIM=1.82E-01), the time interval for printing the output and the integration steps to be used are also specified in the TERMINAL section. There is also the specification for KON2 and KON4 to be set equal to last values of C and H5, respectively. A WRITE statement indicating that values of KON2 and KON4 used for each iteration be printed, is also specified in this section.

4.9.5 Description of the computer program for calculating χ_w, ψ_w, ω_w, χ_s, ψ_s and ω_s for water and salt flow

The governing equations are equations 3.72 through to 3.83 which were all recasted with λ as the independent variable, thus obtaining their corresponding equations shown in Table 4.2a. In recasting with λ as the independent variable, the original definition of P and P_s were used. R and R_s are rewritten as:

$$R(\lambda) = Q(\lambda)\ [2\frac{d\psi_w}{d\lambda}\frac{d\lambda}{d\chi_w} - \frac{d\chi_w}{d\lambda}] \tag{4.116}$$

$$R_s(\lambda) = Q_s(\lambda)\ [2\frac{d\psi_s}{d\lambda}\frac{d\lambda}{d\chi_s} - \frac{d\chi_s}{d\lambda}] \tag{4.117}$$

The advantage with recasting the equations with λ as the independent variable is that experimentally determined values of $c(\lambda)$ and $\theta(\lambda)$

TABLE 4.2a. Recasted Form of the Ordinary Differential Equations 3.72 to 3.83 with λ as the Independent Variable

Water		Solute	
$\chi_w \frac{d\theta}{d\lambda} = \frac{d}{d\lambda}[D \frac{d\theta}{d\lambda} \frac{d\chi_w}{d\lambda}] + \frac{dK}{d\lambda}$	(4.118)	$(\theta\chi_s - D \frac{d\theta}{d\lambda} \frac{d\chi_w}{d\lambda} - K) \frac{dc}{d\lambda} = \frac{d}{d\lambda}[\theta D_s \frac{dc}{d\lambda} \frac{d\chi_s}{d\lambda}]$	(4.119)
$\frac{3}{2} \psi_w \frac{d\theta}{d\lambda} = \frac{d}{d\lambda}[D \frac{d\theta}{d\lambda} \frac{d\psi_w}{d\lambda} - Q]$	(4.120)	$(\frac{3}{2}\theta\psi_s - D \frac{d\theta}{d\lambda} \frac{d\psi_w}{d\lambda} + Q) \frac{dc}{d\lambda} = \frac{d}{d\lambda}[\theta D_s \frac{dc}{d\lambda} \frac{d\psi_s}{d\lambda} - Q_s]$	(4.121)
$2\omega_w \frac{d\theta}{d\lambda} = \frac{d}{d\lambda}[D \frac{d\theta}{d\lambda} \frac{d\omega_w}{d\lambda} - R]$	(4.122)	$(2\theta\omega_s - D \frac{d\theta}{d\lambda} \frac{d\omega_w}{d\lambda} + R) \frac{dc}{d\lambda} = \frac{d}{d\lambda}[\theta D_s \frac{dc}{d\lambda} \frac{d\omega_s}{d\lambda} - R_s]$	(4.123)

TABLE 4.3. Initial and Boundary Conditions for Equations 4.118 to 4.123

Equation	Initial and Boundary Conditions	
4.118	$\lambda=0,\ \theta=\theta_o,\ \chi_w=0$	4.124a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ D\frac{d\theta}{d\lambda}\frac{d\chi_w}{d\lambda}=0$	4.124b
4.119	$\lambda=0,\ \theta=\theta_o,\ c=c_o,\ \chi_s=0$	4.125a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ c=c_n,\ \theta D_s\frac{dc}{d\lambda}\frac{d\chi_s}{d\lambda}=0$	4.125b
4.120	$\lambda=0,\ \theta=\theta_o,\ \psi_w=0$	4.126a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ D\frac{d\theta}{d\lambda}\frac{d\psi_w}{d\lambda}-Q=0,\ Q=0$	4.126b
4.121	$\lambda=0,\ \theta=\theta_o,\ c=c_o,\ \psi_s=0$	4.127a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ c=c_n,\ \theta D_s\frac{dc}{d\lambda}\frac{d\psi_s}{d\lambda}-Q_s=0,\ Q_s=0$	4.127b
4.122	$\lambda=0,\ \theta=\theta_o,\ \omega_w=0$	4.128a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ D\frac{d\theta}{d\lambda}\frac{d\omega_w}{d\lambda}-R=0,\ R=0$	4.128b
4.123	$\lambda=0,\ \theta=\theta_o,\ c=c_o,\ \omega_s=0$	4.129a
	$\lambda=\lambda_n,\ \theta=\theta_n,\ c=c_n,\ \theta D_s\frac{dc}{d\lambda}\frac{d\omega_s}{d\lambda}-R_s=0,\ R_s=0$	4.129b

can be used to calculate D, D_s, χ_w, ψ_w, ω_w, χ_s, ψ_s and ω_s and hence compute the moisture content and concentration profiles for different time periods. Alternatively, if D(θ) and θD_s values are available, θ(λ) and c(λ) can be simulated using the program outlined in figure 4.6 and then calculate χ, ψ and ω for both water and salt flow. The relation between θ and χ is not unique. Consequently, recasting the equations with θ as the independent variable presents problems with computer simulation.

The initial and boundary conditions used to solve equations 4.118 to 4.123 are given in Table 4.3. The terms in brackets on the righthand side of equations 4.118 to 4.123 are designated y_1, y_2, y_3, etc. so that we have:

$$y_1 = D(\theta) \frac{d\theta}{d\lambda} \frac{d\chi_w}{d\lambda} \tag{4.130}$$

$$y_2 = \theta D_s \frac{dc}{d\lambda} \frac{d\chi_s}{d\lambda} \tag{4.131}$$

$$y_3 = D \frac{d\theta}{d\lambda} \frac{d\psi_w}{d\lambda} - Q \tag{4.132}$$

$$y_4 = \theta D_s \frac{dc}{d\lambda} \frac{d\psi_s}{d\lambda} - Q_s \tag{4.133}$$

$$y_5 = D \frac{d\theta}{d\lambda} \frac{d\omega_w}{d\lambda} - R \tag{4.134}$$

$$y_6 = \theta D_s \frac{dc}{d\lambda} \frac{d\omega_s}{d\lambda} - R_s \tag{4.135}$$

which upon substitution into equations 4.118 to 4.123 yield:

$$\frac{dy_1}{d\lambda} = \chi_w \frac{d\theta}{d\lambda} - \frac{dK}{d\lambda} \qquad (4.136)$$

$$\frac{dy_2}{d\lambda} = (\theta\chi_s - D \frac{d\theta}{d\lambda} \frac{d\chi_w}{d\lambda} - K) \frac{dc}{d\lambda} \qquad (4.137)$$

$$\frac{dy_3}{d\lambda} = \frac{3}{2} \psi_w \frac{d\theta}{d\lambda} \qquad (4.138)$$

$$\frac{dy_4}{d\lambda} = (\frac{3}{2} \theta\psi_s - D \frac{d\theta}{d\lambda} \frac{d\psi_w}{d\lambda} + Q) \frac{dc}{d\lambda} \qquad (4.139)$$

$$\frac{dy_5}{d\lambda} = 2\omega_w \frac{d\theta}{d\lambda} \qquad (4.140)$$

$$\frac{dy_6}{d\lambda} = (2\theta\omega_s - D \frac{d\theta}{d\lambda} \frac{d\omega_w}{d\lambda} + R) \frac{dc}{d\lambda} \qquad (4.141)$$

Integration of equations 4.136 to 4.141 with respect to λ yields y_1, y_2, y_3, y_4, y_5 and y_6 which in the computer program written in system 360 CSMP (figure 4.9) are designated RVEL, RVELS, QVEL, QVELS, SVEL and SVELS, respectively. $dy_1/d\lambda$, $dy_2/d\lambda$, $dy_3/d\lambda$, $dy_4/d\lambda$, $dy_5/d\lambda$ and $dy_6/d\lambda$ are also respectively designated RDIV, RDIVS, QDIV, QDIVS, SDIV and SDIVS.

Integrating equations 4.130 to 4.135 and using the initial conditions formulated in equations 4.124a, 4.125a, 4.126a, 4.127a, 4.128a and 4.129a, we obtain:

$$\chi_w = \int_0^\lambda \frac{y_1}{D} \frac{d\lambda}{d\theta} d\lambda \qquad (4.142)$$

$$\chi_s = \int_0^\lambda \frac{y_2}{\theta D_s} \frac{d\lambda}{dc} d\lambda \qquad (4.143)$$

$$\psi_w = \int_0^{\lambda} [(y_3 + Q)/D \frac{d\theta}{d\lambda}] \, d\lambda \tag{4.144}$$

$$\psi_s = \int_0^{\lambda} [(y_4 + Q_s)/\theta D_s \frac{dc}{d\lambda}] \, d\lambda \tag{4.145}$$

$$\omega_w = \int_0^{\lambda} [(y_5 + R)/D \frac{d\theta}{d\lambda}] \, d\lambda \tag{4.146}$$

$$\omega_s = \int_0^{\lambda} [(y_6 + R_s)/\theta D_s \frac{dc}{d\lambda}] \, d\lambda \tag{4.147}$$

As with the preceding programs, the first specification in the computer program used to calculate χ_w, χ_s, ψ_w, ψ_s, ω_w and ω_s (see figure 4.9 and also Appendix H) is to rename time=lambda so that integration and differentiation would be performed with respect to lambda. The INITIAL section then begins with constants specified in CSMP data statements INCON, PARAMETER and CONSTANT, which are all used to assign numerical values. In figure 4.9 the following are assigned numerical values:

(1) RVELN, RVELNS, QVELN, QVELNS, SVELN, SVELNS: equal to y_1, y_2, y_3, y_4, y_5 and y_6, respectively, of equations 4.130 to 4.135, evaluated at $\lambda=\lambda_n$ (FINTIM). These specify the boundary conditions formulated in equations 4.124b, 4.125b, 4.126b, 4.127b, 4.128b and 4.129b.

(2) SEELAO: the derivative of $c(\lambda)$ at $\lambda=0$

(3) SEEO: the concentration of chloride in solution at $\lambda=0$

(4) SEEN: the initial concentration of chloride in the moist soil, c_n

(5) DCONDO: the derivative of hydraulic conductivity as a function of

FIGURE 4.9

CSMP listing for calculating χ, ψ, and ω for water and salt flow (Brookston clay).

```
                 ****CONTINUOUS SYSTEM MODELING PROGRAM****

                            *** VERSION 1.3 ***

TITLE CHI,PSI, AND OMEGA FOR WATER AND SALT FLOW (BROCKSTON CLAY)
*     UNITS
*     KEQ=KILO-EQUIVALENTS
*     KG=KILOGRAMS
*     M=METERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     RVELN=PRODUCT OF SOIL WATER DIFFUSIVITY, DERIVATIVE OF WATER
*     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF CHI OF
*     WATER WITH RESPECT TO LAMBDA AT LAMDAN (=LAMBDA AT FINTIM)
*     QVELN=PRODUCT OF SOIL WATER DIFFUSIVITY, DERIVATIVE OF WATER
*     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF PSI FOR
*     WATER WITH RESPECT TO LAMBDA MINUS Q EVALUATED AT LAMDAN
*     (=LAMBDA AT FINTIM)
*     Q=PRODUCT OF SOIL WATER DIFFUSIVITY ,DERIVATIVE OF WATER
*     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF CHI OF
*     WATER SQUARED
*     R=Q MULTIPLIED BY THE DIFFERENCE BETWEEN TWICE THE DERIVATIVE
*     OF PSI FOR WATER WITH RESPECT TO CHI FOR WATER AND THE
*     DERIVATIVE OF CHI FOR WATER WITH RESPECT TO LAMBDA
*     QS=THE PRODUCT OF WATER CONTENT ,THE DERIVATIVE OF CHLORIDE
*     CONCENTRATION WITH RESPECT TO LAMBDA ,AND THE DERIVATIVE
*     OF CHI FOR SALT WITH RESPECT TO LAMBDA SQUARED
*     RS=QS MULTIPLIED BY THE DIFFERENCE BETWEEN TWICE THE DERIVATIVE
*     OF PSI FOR SALT WITH RESPECT TO CHI FOR SALT AND THE
*     DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
*     SVELN=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE
*     OF WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
*     OMEGA FOR WATER WITH RESPECT TO LAMBDA MINUS R EVALUATED AT
*     LAMDAN (=LAMBDA AT FINTIM)
*     RVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT
*     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO LAMBDA
*     AND THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
*     EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
*     QVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
*     THE DERIVATIVE OF CHLORIDE CONCENTRATION WITH RESPECT TO
*     LAMBDA AND THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO
*     LAMBDA MINUS QS EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
*     SVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
*     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*     LAMBDA AND THE DERIVATIVE OF OMEGA OF SALT WITH RESPECT TO
*     LAMBDA EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
*     SEELAO=DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RWSPECT TO
*     LAMBDA EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
*     SEELO=CHLORIDE CONCENTRATION AT LAMBDA EQUALS ZERO
*     SEEN=INITIAL CHLORIDE CONCENTRATION OF THE MOIST SOIL
*     DCONDO=DERIVATIVE OF THE HYDRAULIC CONDUCTIVITY WITH RESPECT TO
*     LAMBDA EVALUATED AT LAMDAN (=LAMDA AT FINTIM)
*     RVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY,THE DERIVATIVE OF
*     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
*     CHI OF WATER WITH RESPECT TO LAMBDA
*     RVELO=RVEL EVALUATED AT LAMBDA EQUALS ZERO
*     QVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE OF
*     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
*     PSI OF WATER WITH RESPECT TO LAMBDA MINUS Q
*     QVELO=QVEL EVALUATED AT LAMBDA EQUALS ZERO
*     SVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE OF
*     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
*     OMEGA FOR WATER WITH RESPECT TO LAMBDA MINUS R
*     SVELO=SVEL EVALUATED AT LAMBDA EQUALS ZERO
```

```
*     RVELS=THE PRODUCT OF WATER CONTENT, THE DISPERSION COEFFICIENT
*     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*     LAMBDA AND THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO
*     LAMBDA
*     VELO=RVELS EVALUATED AT LAMBDA EQUALS ZERO
*     QVELS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
*     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*     LAMBDA AND THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO
*     LAMBDA MINUS QS
*     QVELOS=QVELS EVALUATED AT LAMBDA EQUALS ZERO
*     SVELS=THE PRODUCT OF THE WATER CONTENT, THE DISPERSION COEFFICIENT
*     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*     LAMBDA AND THE DERIVATIVE OF OMEGA FOR SALT WITH RESPECT TO
*     LAMBDA MINUS RS
*     SVELOS=SVELS EVALUATED AT LAMBDA EQUALS ZERO
*     THLAO=THE DERIVATIVE OF THE WATER CONTENT WITH RESPECT TO
*     LAMBDA EVALUATED AT LAMBDA EQUALS ZERO
*     THETAO=WATER CONTENT AT LAMBDA EQUALS ZERO
*     DPSIO=THE DERIVATIVE OF PSI FOR WATER WITH RESPECT TO LAMBDA
*     EVALUATED AT LAMBDA EQUALS ZERO
*     DCHIO=THE DERIVATIVE OF CHI FOR WATER WITH RESPECT TO LAMBDA
*     EVALUATED AT LAMBDA EQUALS ZERO
*     OMEGAO=THE DERIVATIVE OF OMEGA OF WATER WITH RESPECT TO
*     LAMBDA EVALUATED AT LAMBDA EQUALS ZERO
*     DCHISO=THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
*     EVALUATED AT LAMBDA EQUALS ZERO
*     DPSISO=THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO LAMBDA
*     EVALUATED AT LAMBDA EQUALS ZERO
*     KON2=THE INTEGRAL VALUE OF THE WATER CONTENT FROM LAMBDA EQUALS
*     ZERO TO LAMBDAN (=LAMBDA AT FINTIM)
*     G=THE SUM OF THETA TIMES LAMBDA AND TWICE THE SOIL WATER
*     DIFFUSIVITY MULTIPLIED BY THE DERIVATIVE OF WATER CONTENT WITH
*     RESPECT TO LAMBDA
*     KON3=THE INTEGRAL VALUE OF THE PRODUCT OF G AND THE DERIVATIVE
*     OF THE CHLORIDE CONCENTRATION WITH RESPECT TO LAMBDA FROM
*     LAMBDA EQUALS ZERO TO LAMDAN (=LAMBDA AT FINTIM)
*     THETAN=INITIAL SOIL WATER CONTENT
*     SEE=TABLE OF CHLORIDE CONCENTRATION VERSUS LAMBDA
*     THETA=TABLE OF WATER CONTENT VERSUS LAMBDA
*     COND=TABLE OF HYDRAULIC CONDUCTIVITY VERSUS WATER CONTENT
*     THLA=LINEAR INTERPOLATION OF THETA-LAMBDA EXPERIMENTAL DATA
*     PROVIDED IN FUNCTION THETA
*     SEELA=LINEAR INTERPOLATION OF EXPERIMENTAL CONCENTRATION
*     VERSUS LAMBDA DATA PROVIDED IN FUNCTION SEE
*     HCOND=NON-LINEAR INTERPOLATION OF HYDRAULIC CONDUCTIVITY
*     VERSUS LAMBDA THROUGH THE DERIVED HYDRAULIC CONDUCTIVITY VERSUS
*     THETA PROVIDED IN FUNCTION COND
*     A=DERIVATIVE OF WATER CONTENT WITH RESPECT TO LAMBDA
*     C=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO LAMDAN
*     (=LAMBDA AT FINTIM)
*     D=SOIL WATER DIFFUSIVITY
*     CTHETA=DIMENSIONLESS WATER CONTENT
*     CSEE=DIMENSIONLESS CHLORIDE CONCENTRATION
*     CI=THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT
*     TO LAMBDA
*     DS=DISPERSION COEFFICIENT
*     THDS=THE PRODUCT OF THE WATER CONTENT AND THE DISPERSION
*     COEFFICIENT
*     RDIV=THE DERIVATIVE OF Y1 WITH RESPECT TO LAMBDA IN EQUATION 4.136
*     QDIV=THE DERIVATIVE OF Y3 WITH RESPECT TO LAMBDA IN EQUATION 4.138
*     SDIV=THE DERIVATIVE OF Y5 WITH RESPECT TO LAMBDA IN EQUATION 4.140
*     RDIVS=THE DERIVATIVE OF Y2 WITH RESPECT TO LAMBDA IN EQUATION 4.137
*     QDIVS=THE DERIVATIVE OF Y4 WITH RESPECT TO LAMBDA IN EQUATION 4.139
*     SDIVS=THE DERIVATIVE OF Y6 WITH RESPECT TO LAMBDA IN EQUATION 4.141
*     CHI=CHI FOR WATER
*     PSI=PSI FOR WATER
```

```
*     OMEGA=OMEGA FOR WATER
*     CHIS=CHI FOR SALT
*     PSIS=PSI FOR SALT
*     OMEGAS=OMEGA FOR SALT
  RENAME TIME=LAMDA
INITIAL
          INCON DEL=.00001,RVELN=0.0,QVELN=0.0,SVELN=0.0,...
          RVELNS=0.0,QVELNS=0.0,SVELNS=0.0,...
          SEELAO=-1.0,SEEO=.97,SEEN=.00018,DCONDO=-6.9615E-03,...
          RVELO=-.326814E-05,QVELO=.5200022E-08,SVELO=.1214903E-10,...
          VELO=-.5948184E-07,QVELCS=-.2270695E-10,SVELCS=.7740965E-13
          PARAMETER THLAO=-5.0,THETAO=.53,LAMDAN=1.82E-03,...
          DCHIO=.98621E-02,DPSIO=8.3099E-05,OMEGAO=.63819E-06,...
          DCHISO=2.2168E-03,DPSISO=5.761E-06
          CONSTANT THETAN=.12,KON2=1.0,KON3=1.0,I=0,J=0
          FUNCTION THETA=(0.0,.53),(1.0E-04,.525),(3.0E-04,.52),...
          (5.0E-04,.515),(7.0E-04,.51),(9.0E-04,.50),(1.0E-03,.495),...
          (1.1E-03,.49),(1.2E-03,.48),(1.3E-03,.473),(1.4E-03,.463),...
          (1.5E-03,.445),(1.55E-03,.435),(1.6E-03,.42),(1.65E-03,.40),...
          (1.7E-03,.37),(1.75E-03,.325),(1.78E-03,.28),(1.8E-03,.235),...
          (1.81E-03,.185),(1.82E-03,.12),(1.9E-03,.12),(2.0E-03,.12)
          FUNCTION SEE=(0.0,.97),(1.0E-04,.9699),(2.0E-04,.9698),...
          (3.0E-04,.9697),(4.0E-04,.9696),(5.0E-04,.9695),...
          (6.0E-04,.9694),(7.0E-04,.9693),(8.0E-04,.9692),...
          (9.0E-04,.96),(1.0E-03,.95),(1.1E-03,.93),(1.2E-03,.895),...
          (1.25E-03,.87),(1.3E-03,.825),(1.35E-03,.765),...
          (1.4E-03,.64),(1.42E-03,.54),(1.43E-03,.49),(1.44E-03,.40),...
          (1.45E-03,.35),(1.46E-03,.30),(1.47E-03,.25),(1.48E-03,.20),...
          (1.49E-03,.18),(1.50E-03,.15),(1.52E-03,.12),(1.54E-03,.09),...
          (1.55E-03,.085),(1.56E-03,.075),(1.57E-03,.065),...
          (1.58E-03,.06),(1.595E-03,.05),(1.615E-03,.04),...
          (1.63E-03,.03),(1.65E-03,.025),(1.67E-03,.02),(1.7E-3,.015),...
          (1.75E-03,.01),(1.82E-03,.005),(1.9E-03,.001),(2.0E-3,0.0)
          FUNCTION COND=(.12,1.56E-09),(.161,2.0E-09),(.202,2.72E-09),...
          (.243,4.0E-09),(.284,6.72E-09),(.325,1.6E-08),(.366,6.4E-08),...
          (.3824,1.0E-07),(.407,1.92E-07),(.4234,2.84E-07),...
          (.448,4.8E-07),(.4726,8.8E-07),(.489,1.44E-06),...
          (.5136,2.88E-06),(.53,4.8E-06)
          RVELAO=RVELO*(1.0+DEL)
          QVELAO=QVELO*(1.0+DEL)
          SVELAO=SVELO*(1.0+DEL)
          VELAO=VELO*(1.0+DEL)
          QLAOS=QVELOS*(1.0+DEL)
          VELSAO=SVELCS*(1.0+DEL)
DYNAMIC
          THLA=AFGEN(THETA,LAMDA)
          HCOND=NLFGEN(COND,THLA)
          DHCOND=DERIV(DCONDO,HCOND)
          A=DERIV(THLAO,THLA)
          C=INTGRL(0.0,THLA)
          KON1=LAMDAN*THETAN
          E=(THLA*LAMDA)-KON1
          FF=E-C
          G=FF+KON2
          D=-.5*G/A
          CTHETA=(THLA-THETAN)/(THETAO-THETAN)
          CSEE=(SEELA-SEEN)/(SEEO-SEEN)
          SEELA=AFGEN(SEE,LAMDA)
          C1=DERIV(SEELAO,SEELA)
          LATHH=(THLA*LAMDA)+(2.0*D*A)
          GS=C1*LATHH
          HS=INTGRL(0.0,GS)
          HS1=KON3-HS
          THDS=.5*HS1/C1
          DS=THDS/THLA
          NOSORT
```

```
          IF(J.LE.3) GO TO 10
          IF(THDS.EQ.0.0) GO TO 10
          SORT
          RDIV=(CHI*A)-DHCOND
          RDIVA=(CHIA*A)-DHCOND
          RVEL=INTGRL(RVELO,RDIV)
          RVELA=INTGRL(RVELAO,RDIVA)
          B1=RVEL/(D*A)
          BB1=RVELA/(D*A)
          CHI=INTGRL(0.0,B1)
          CHIA=INTGRL(0.0,BB1)
          DDCHI=DERIV(DCHIO,CHI)
          Q=D*A*DDCHI*DDCHI
          QDIV=1.5*PSI*A
          QDIVA=1.5*PSIA*A
          QVEL=INTGRL(QVELO,QDIV)
          QVELA=INTGRL(QVELAO,QDIVA)
          CC1=(QVEL+Q)/(A*D)
          CC2=(QVELA+Q)/(A*D)
          PSI=INTGRL(0.0,CC1)
          PSIA=INTGRL(0.0,CC2)
          DPSI=DERIV(DPSIO,PSI)
          CC3=(2.0*DPSI/DDCHI)-DDCHI
          R=Q*CC3
          SDIV=2.0*OMEGA*A
          SDIVA=2.0*OMEGAA*A
          SVEL=INTGRL(SVELO,SDIV)
          SVELA=INTGRL(SVELAO,SDIVA)
          DD1=(SVEL+R)/(A*D)
          DD2=(SVELA+R)/(A*D)
          OMEGA=INTGRL(0.0,DD1)
          OMEGAA=INTGRL(0.0,DD2)
          DOMEGA=DERIV(OMEGAO,OMEGA)
          RDIVS=((THLA*CHIS)-(D*A*DDCHI)-HCOND)*C1
          RDIVAS=((THLA*CHIAS)-(D*A*DDCHI)-HCOND)*C1
          RVELS=INTGRL(VELO,RDIVS)
          RVELAS=INTGRL(VELAO,RDIVAS)
          BB=RVELS/(THDS*C1)
          BBA=RVELAS/(THDS*C1)
          CHIS=INTGRL(0.0,BB)
          CHIAS=INTGRL(0.0,BBA)
          DCHIS=DERIV(DCHISO,CHIS)
          QS=THDS*C1*DCHIS*DCHIS
          QDIVS=((1.5*THLA*PSIS)-(D*A*DPSI)+Q)*C1
          QDIVAS=((1.5*THLA*PSIAS)-(D*A*DPSI)+Q)*C1
          QVELS=INTGRL(QVELOS,QDIVS)
          QVELAS=INTGRL(QVELAOS,QDIVAS)
          CC=(QVELS+QS)/(THDS*C1)
          CCA=(QVELAS+QS)/(THDS*C1)
          PSIS=INTGRL(0.0,CC)
          PSIAS=INTGRL(0.0,CCA)
          DPSIS=DERIV(DPSISO,PSIS)
          RS=QS*((2.0*DPSIS/DCHIS)-DCHIS)
          SDIVS=((2.0*THLA*OMEGAS)-(D*A*DOMEGA)+R)*C1
          SDIVAS=((2.0*THLA*MEGAAS)-(D*A*DOMEGA)+R)*C1
          SVELS=INTGRL(SVELOS,SDIVS)
          SVELAS=INTGRL(VELSAO,SDIVAS)
          DD=(SVELS+RS)/(THDS*C1)
          DDA=(SVELAS+RS)/(THDS*C1)
          OMEGAS=INTGRL(0.0,DD)
          MEGAAS=INTGRL(0.0,DDA)
          NOSORT
   10     CONTINUE
TERMINAL
          METHOD SIMP
          TIMER FINTIM=1.82E-03,PRDEL=3.64E-05,DELT=1.0E-05
```

```
         PRINT CTHETA,CHI,PSI,CMEGA,CSEE,CHIS,PSIS,OMEGAS
         IF(J.GE.4) GC TO 15
         J=J+1
         KON2=C
         KON3=HS
         GO TO 2C
   15    I=I+1
         IF(ABS(RVELN-RVEL).EG.0.0) STCP
         IF(ABS(QVELN-QVEL).EG.C.C) STOP
         IF(ABS(SVELN-SVEL).EG.0.C) STCP
         IF(ABS(RVELNS-RVELS).EQ.0.0) STCP
         IF(ABS(QVELNS-QVELS).EQ.0.0) STCP
         IF(ABS(SVELNS-SVELS).EQ.0.0) STCP
         DVEL=RVELA-RVEL
         DVEL1=QVELA-QVEL
         DVEL2=SVELA-SVEL
         DVELS=RVELAS-RVELS
         DVELS1=QVELAS-QVELS
         DVELS2=SVELAS-SVELS
         SLOPE=DVEL/DEL/RVELO
         SLOPE1=DVEL1/DEL/QVELC
         SLOPE2=DVEL2/DEL/SVELC
         RSLOPE=DVELS/DEL/VELC
         QSLOPE=DVELS1/DEL/QVELCS
         SSLOPE=DVELS2/DEL/SVELCS
         DRVEL=(RVELN-RVEL)/SLCPE
         DQVEL=(QVELN-QVEL)/SLCPE1
         DSVEL=(SVELN-SVEL)/SLCPE2
         DRVELS=(RVELNS-RVELS)/RSLOPE
         DQVELS=(QVELNS-QVELS)/QSLOPE
         DSVELS=(SVELNS-SVELS)/SSLOPE
         RVELO=RVELO+DRVEL
         QVELO=QVELO+DQVEL
         SVELO=SVELO+DSVEL
         VELO=VELO+DRVELS
         QVELOS=QVELCS+DQVELS
         SVELOS=SVELCS+DSVELS
         RVELAO=RVELO*(1.0+DEL)
         QVELAO=QVELC*(1.0+DEL)
         SVELAO=SVELO*(1.0+DEL)
         VELAO=VELO*(1.0+DEL)
         QLAOS=QVELOS*(1.0+DEL)
         VELSAO=SVELOS*(1.0+DEL)
         WRITE(6,101) RVELC,RVELAC
  101    FORMAT(//' CALL RERUN WITH RVELC,RVELAO=',2E2C.7)
         WRITE(6,102) QVELO,QVELAO
  102    FORMAT(//' CALL RERUN WITH QVELC,QVELAO=',2E20.7)
         WRITE(6,103) SVELO,SVELAO
  103    FORMAT(//' CALL RERUN WITH SVELC,SVELAO=',2E20.7)
         WRITE(6,104) VELO,VELAO
  104    FORMAT(//' CALL RERUN WITH VELO,VELAO=',2E20.7)
         WRITE(6,105) QVELCS,CLACS
  105    FORMAT(//' CALL RERUN WITH QVELCS,QLAOS=',2E20.7)
         WRITE(6,106) SVELOS,VELSAO
  106    FORMAT(//' CALL RERUN WITH SVELCS,VELSAO=',2E2C.7)
   20    IF(J.GT.15) STOP
         IF(I.GT.13) STCP
         CALL PERUN
      END
      STOP
```

lambda evaluated at $\lambda=0$

(6) RVELO, VELO, QVELO, QVELOS, SVELO, SVELOS: are y_1, y_2, y_3, y_4, y_5 and y_6, respectively, evaluated at $\lambda=0$. These values are initially estimated and the algorithm in the TERMINAL section calculates actual values which ensure that the boundary conditions stipulated in equations 4.124b, 4.125b, 4.126b, 4.127b, 4.128b and 4.129b in the TERMINAL section are satisfied.

(7) THLAO: the derivative of $\theta(\lambda)$ estimated at $\lambda=0$

(8) THETAO: moisture content at $\lambda=0$

(9) LAMDAN: FINTIM lambda, i.e. λ_n or λ_F

(10) DCHIO, DPSIO, OMEGAO: are respectively, $d\chi_w/d\lambda$, $d\psi_w/d\lambda$, $d\omega_w/d\lambda$ evaluated at $\lambda=0$

(11) DCHISO, DPSISO: are, respectively, $d\chi_s/d\lambda$, $d\psi_s/d\lambda$ at $\lambda=0$

(12) THETAN: initial water content of the moist soil

(13) KON2: the definite integral $\int_0^{\lambda_F} \theta d\lambda$

(14) KON3: the definite integral $\int_0^{\lambda_F} g(\theta)\frac{dc}{d\lambda}\, d\lambda$

The use of KON2 and KON3 has been explained in section 4.9.2 which deals with simulation of $c(\lambda)$ from calculated $D(\lambda)$ and $D_s(\lambda)$ values. RVELO, VELO, QVELO, QVELOS, SVELO, and SVELOS are each multiplied by 1.00001 thus obtaining RVELAO, VELAO, QVELAO, QLAOS, SVELAO and VELSAO which are the initial values of the half pair of y_1, y_2, y_3, y_4, y_5 and y_6. Tables of concentration versus lambda (FUNCTION SEE), moisture content versus lambda (FUNCTION THETA) and hydraulic conductivity versus moisture content (FUNCTION COND) are provided. In these tables values of the independent variable, for example lambda in the case of FUNCTIONS SEE and THETA, are listed first in the brackets with the corresponding dependent variable.

The DYNAMIC section consists basically of seven subprograms which are executed through the sorting capability of CSMP algorithm. The first subroutine calculates the moisture diffusivity D and then the dispersion coefficient D_s and is similar to the program already described in section 4.9.2. An IF statement after the statement for calculating the D_s (figure 4.9) ensures that at least three iterations are carried out to obtain the correct D and D_s values to be used in the other six subroutines.

The second subroutine calculates χ_w. $dy_1/d\lambda$ in equation 4.136 is designated RDIV and equation 4.108 written in CSMP statement form as:

```
RDIV = (CHI*A) - DHCOND                                    (4.148)
```

Here, DHCOND as already specified in the first subroutine is the derivative of the hydraulic conductivity with respect to λ done through the statements:

```
 HCOND = NLFGEN(COND, THLA)                               (4.149a)
DHCOND = DERIV(DCONDO, HCOND)                             (4.149b)
```

Integration of RDIV gives y_1 which is designated RVEL:

```
RVEL  = INTGRL (RVELO, RDIV)                               (4.150)
```

In equation 4.150, RVELO which is the value of y_1 at $\lambda=0$ is not known and so a guess is first made. The integrand in equation 4.142 designated B1 is then calculated through the statement:

B1 = RVEL/(D*A) (4.151)

B1 is then integrated to obtain χ_w through the statement:

CHI = INTGRL(0.0, B1) (4.152)

RDIV, RVEL, B1 and CHI are paired using the multiplying factor 1.00001 to obtain RVELAO as specified in the INITIAL segment of the program. The following statements are the half pairs of RDIV, RVEL, B1 and CHI:

RDIVA = (CHIA*A) - DHCOND (4.153)

RVELA = INTGRL(RVELAO, RDIVA) (4.154)

BB1 = RVELA/(D*A) (4.155)

CHIA = INTGRL(0.0, BB1) (4.156)

At this stage the derivative of χ_w, (i.e. $d\chi_w/d\lambda$) is calculated using the statement:

DDCHI = DERIV(DCHIO, CHI) (4.157)

This is followed by calculation of Q in equation 4.120 and defined in 3.80:

Q = D*A*DDCHI*DDCHI (4.158)

The third subroutine calculates ψ_w. $dy_3/d\lambda$ in equation 4.138 is designated QDIV and equation 4.138 written in a CSMP statement as:

QDIV = 1.5*PSI*A (4.159)

Integration of QDIV yields y_3 which is designated QVEL:

QVEL = INTGRL(QVELO, QDIV) (4.160)

The integrand in equation 4.144 designated CC1 is calculated by the statement:

CC1 = (QVEL+Q)/(A*D) (4.161)

CC1 is then integrated to obtain ψ_w through the statement:

PSI = INTGRL(0.0, CC1) (4.162)

As was done with the second subroutine, QDIV, QVEL, CC1 and PSI in this third subroutine are also paired through the multiplier 1.00001 used to obtain QVELAO from QVELO. The half pairs are:

QDIVA = 1.5*PS1A*A (4.163)

QVELA = INTGRL(QVELAO, QDIVA) (4.164)

```
CC2  =  (QVELA+Q)/(A*D)                                   (4.165)

PS1A =  INTGRL(0.0, CC2)                                  (4.166)
```

The derivative of ψ_w with respect to λ designated DPS1 and then R in equation 4.122 (defined in equation 3.82) are respectively calculated as follows:

```
DPS1 =  DERIV(DPS10, PS1)                                 (4.167)

CC3  =  (2.0*DPS1/DDCHI) - DDCHI                          (4.168)

R    =  Q*CC3                                             (4.169)
```

The fourth subroutine calculates ω_w . $dy_5/d\lambda$ in equation 4.140 is designated SDIV and equation 4.140 written as:

```
SDIV =  2.0*OMEGA*A                                       (4.170)
```

Equation 4.170 is integrated to obtain y_5 designated SVEL:

```
SVEL =  INTGRL(SVELO, SDIV)                               (4.171)
```

The integrand in equation 4.146 is calculated with the statement:

```
DD1  =  (SVEL+R)/(A*D)                                    (4.172)
```

Integration of DD1 gives ω_w:

```
OMEGA = INTGRL(0.0, DD1)                                  (4.173)
```

SDIV, SVEL, DD1 and OMEGA are paired as was done with the preceding subroutines as follows:

```
SDIVA  = 2.0*OMEGAA*A                                    (4.174)
SVELA  = INTGRL(SVELAO, SDIVA)                           (4.175)
DD2    = (SVELA+R)/(A*D)                                 (4.176)
OMEGAA = INTGRL(0.0, DD2)                                (4.177)
```

$\frac{d\omega_w}{d\lambda}$ is calculated through the statement:

```
DOMEGA = DERIV(OMEGAO, OMEGA)                            (4.178)
```

The fifth, sixth and seventh subroutines calculate χ_s, ψ_s and ω_s, respectively.

$dy_2/d\lambda$ in equation 4.137 is calculated with the statement:

```
RDIVS = ((THLA*CHIS)-(D*A*DDCH1)-HCOND)*C1               (4.179)
```

Integrating RDIVS gives y_2:

```
RVELS = INTGRL(VELO, RDIVS)                              (4.180)
```

The integrand in equation 4.143 designated BB is calculated and then integrated to obtain χ_s:

```
BB     =  RVELS/(THDS*C1)                          (4.181)

CHIS   =  INTGRL(0.0, BB)                          (4.182)
```

The half pairs of RDIVS, RVELS, BB and CHIS are obtained through VELAO which is 1.00001 multiplied by VELO:

```
RDIVAS = ((THLA*CHIAS)-(D*A*DDCHI)-HCOND)*C1       (4.183)

RVELAS = INTGRL(VELAO, RDIVAS)                     (4.184)

BBA    = RVELAS/(THDS*C1)                          (4.185)

CHIAS  = INTGRL(0.0, BBA)                          (4.186)
```

$d\chi_s/d\lambda$ and Q_s defined in equation 3.81 are computed using the statements:

```
DCHIS  = DERIV(DCHISO, CHIS)                       (4.187)

QS     = THDS*C1*DCHIS*DCHIS                       (4.188)
```

Equation 4.189 calculates $dy_4/d\lambda$ which when integrated (equation 4.190) gives y_4 which is designated QVELS:

```
QDIVS = ((1.5*THLA*PSIS)-(D*A*DPS1)+Q)*C1          (4.189)

QVELS = INTGRL(QVELOS, QDIVS)                      (4.190)
```

The integrand in equation 4.145 is computed and integrated to obtain ψ_s through the statements:

```
CC     = (QVELS+QS)/(THDS*C1)                      (4.191)
```

```
PSIS   =  INTGRL(0.0, CC)                                    (4.192)
```

The half pairs of QDIVS, QVELS, CC and PSIS given by QLAOS are:

```
QDIVAS = ((1.5*THLA*PSIAS)-(D*A*DPS1)+Q)*C1                  (4.193)
QVELAS = INTGRL(QLAOS, QDIVAS)                               (4.194)
CCA    = (QVELAS+QS)/(THDS*C1)                               (4.195)
PSIAS  = INTGRL(0.0, CCA)                                    (4.196)
```

The derivative of ψ_s with respect to λ, $d\psi_s/d\lambda$ and R_s defined in equation 3.83 and recasted with λ as the independent variable in equation 4.117 are computed through the statements:

```
DPSIS  = DERIV(DPSISO,PSIS)                                  (4.197)
RS     = QS*((2.0*DPSIS/DCHIS)-DCHIS)                        (4.198)
```

Equation 4.141 with $dy_6/d\lambda$ designated SDIVS, is computed for each λ step and then integrated through the statements:

```
SDIVS  = ((2.0*THLA*OMEGAS)-(D*A*DOMEGA)+R)*C1               (4.199)
SVELS  = INTGRL(SVELOS,SDIVS)                                (4.200)
```

The integrand in equation 4.147 is computed and then integrated to obtain ω_s as follows:

```
DD     = (SVELS+RS)/(THDS*C1)                                (4.201)
```

OMEGAS = INTGRL(0.0, DD) (4.202)

Using VELSAO (=SVELOS*1.00001) the half pairs of SDIVS, SVELS, DD and OMEGAS are obtained with the statements:

SDIVAS = ((2.0*THLA*MEGASS)-(D*A*DOMEGA)+R)*C1 (4.203)

SVELAS = INTGRL(VELSAO, SDIVAS) (4.204)

DDA = (SVELAS+RS)/(THDS*C1) (4.205)

MEGAAS = INTGRL(0.0, DDA) (4.206)

In the TERMINAL section of figure 4.9 the stipulation is made that Simpson's integration method should be used to perform all integrations. The total simulation time (FINTIM=$1.82\text{x}10^{-3}$), the time interval for printing the output, and the integration step DELT are also specified. An IF statement then enables computation of the first three iterations to be performed with KON2 set equal to the last value of C and KON3 equal to the value of HS at FINTIM. For iterations greater than or equal to 4, the algorithm for computation of new values of RVELO, QVELO, SVELO, VELO, QVELOS and SVELOS for the next iteration is used. This algorithm is similar to that used for the simulation of $\theta(\lambda)$ and $c(\lambda)$, details of which are outlined in Appendices C and D. The boundary conditions formulated in equations 4.124b, 4.125b, 4.126b, 4.127b, 4.128b and 4.129b are specified in an IF statement, requiring computation to stop if the simulated y_1, y_2, y_3, y_4, y_5 and y_6 at FINTIM ($\lambda=1.82\text{x}10^{-3}$) is zero. The rest of the algorithm first calculates the difference between the pair RVELA and RVEL (the other subroutines are similar, for example

DEVLI = QVELA-QVEL). This difference, designated DVEL is divided by 0.00001xRVELO to obtain the slope. The difference between 0.0 and the computed y_1 at FINTIM divided by the slope gives the correction factor DRVEL which is added to the value of RVELO from the preceding iteration to get a new RVELO for subsequent iteration. Similarly, DVEL1, DVEL2, DVELS1 and DVELS2 are the differences between QVELA and QVEL, SVELA and SVEL, RVELAS and RVELS, QVELAS and QVELS, SVELAS and SVELS, respectively. DVEL1, DVEL2, DVELS, DVELS1 and DVELS2 are divided by DEL multiplied by QVELO, SVELO, VELO, QVELOS and SVELOS, respectively, (DEL=.00001) to obtain SLOPE1, SLOPE2, RSLOPE, QSLOPE and SSLOPE which are used to calculate the correction factors DQVEL, DSVEL, DRVELS, DQVELS, DSVELS (see TERMINAL section of figure 4.9). New values of QVELO, SVELO, VELO, QVELOS and SVELOS are thus computed and used for subsequent simulation by adding the correction terms to the preceding values of QVELO, SVELO, etc.

Six WRITE statements specify to the computer to print values of RVELO, RVELAO, QVELO, QVELAO, SVELO, SVELAO, VELO, VELAO, QVELOS, QLAOS, SVELOS and VELSAO used for each iteration following the previous simulation. The last statement enables simulation to be halted if after 13 iterations simulated y_1, y_2, y_3, y_4, y_5 or y_6 at FINTIM fails to converge to zero.

4.9.6 Description of CSMP program for simulating water content profiles for various time periods for vertical infiltration of water and salt

The governing equation is equation 3.68. The actual program written in system 360 CSMP is given in figure 4.10 (see also Appendix I for program

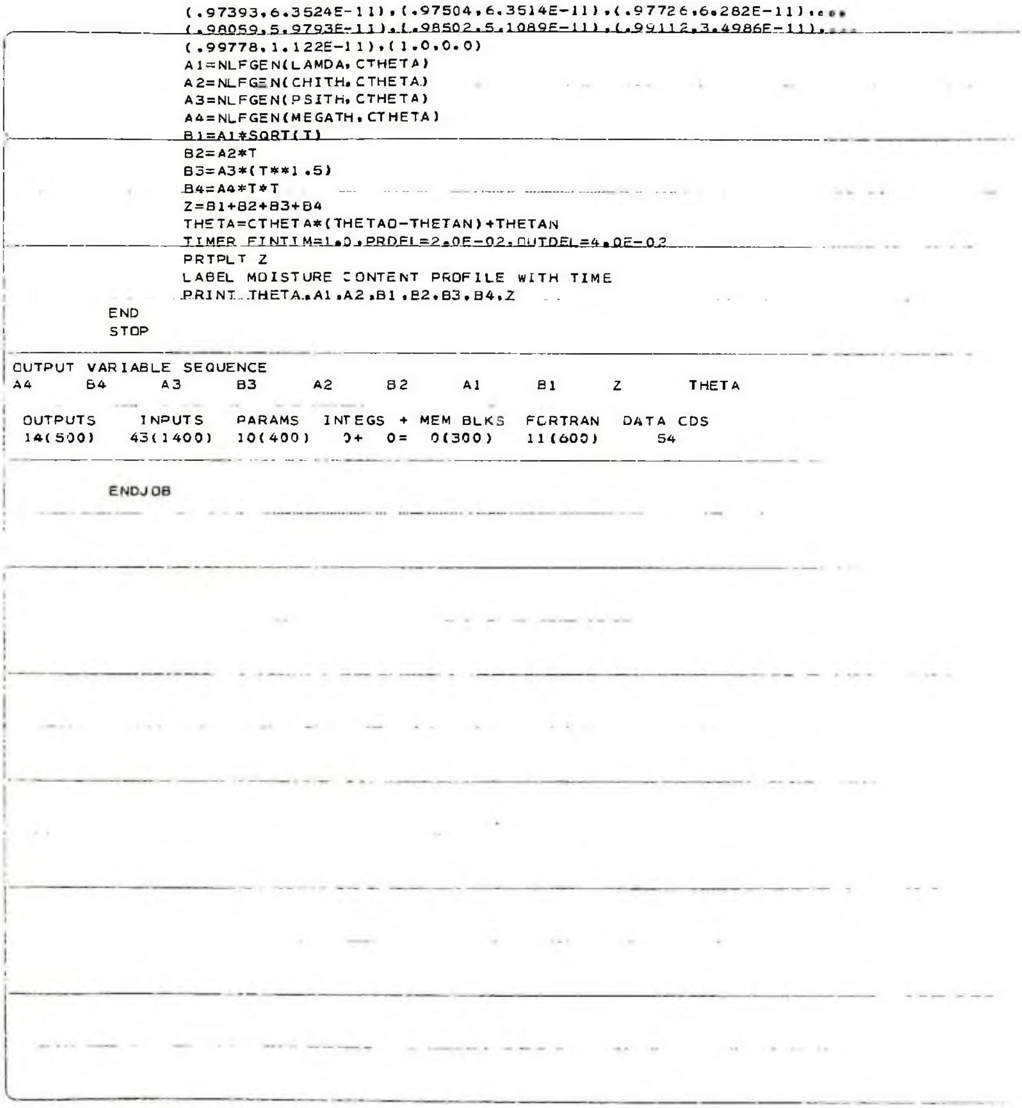
FIGURE 4.10

CSMP listing for simulating water content profiles for various time periods for vertical infiltration of water and salt (Brookston clay).

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                             *** VERSION 1.3 ***

TITLE SOIL WATER CONTENT PROFILE WITH TIME (BROOKSTON CLAY)
*     UNITS
*     KG=KILOGRAMS
*     M=METERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     CTHETA=DIMENSIONLESS WATER CONTENT
*     THETAO=SOIL WATER CONTENT AT LAMBDA EQUALS ZERO, CHI EQUALS ZERO,
*     PSI EQUALS ZERO, AND OMEGA EQUALS ZERO
*     THETAN=INITIAL SOIL WATER CONTENT
*     T=TIME
*     THETA=SOIL WATER CONTENT
*     LAMDA=TABLE OF LAMBDA AND CORRESPONDING WATER CONTENT VALUES
*     CHITH=TABLE OF CHI FOR WATER AND CORRESPONDING WATER CONTENT VALUES
*     PSITH=TABLE OF PSI FOR WATER AND CORRESPONDING WATER CONTENT VALUES
  RENAME TIME=CTHETA
      INCON THETAO=.53,THETAN=.12
      PARAMETER T=(360.0,7200.0,19260.0,21600.0)
      FUNCTION LAMDA=(0.0,1.82E-03),(.1585,1.81E-03),...
      (.2805,1.8E-03),(.3902,1.78E-03),(.5,1.75E-03),...
      (.6098,1.7E-03),(.6829,1.65E-03),(.7317,1.6E-03),...
      (.7683,1.55E-03),(.7927,1.5E-03),(.8366,1.4E-03),...
      (.86098,1.3E-03),(.8781,1.2E-03),(.9024,1.1E-03),...
      (.9146,1.0E-03),(.9268,9.0E-04),(.9512,7.0E-04),...
      (.9634,5.0E-04),(.9756,3.0E-04),(.9878,1.0E-04),...
      (1.0,0.0)
              FUNCTION CHITH=(0.0,3.5179E-06),(.25854,3.4167E-06),...
      (.37049,3.486E-06),(.44366,3.5546E-06),(.50615,3.6234E-06),...
      (.5461,3.6914E-06),(.58605,3.7584E-06),(.64722,3.8887E-06),...
      (.69463,4.0122E-06),(.73015,4.1282E-06),(.75717,4.2365E-06),...
      (.77863,4.3375E-06),(.79602,4.4324E-06),(.812,4.5211E-06),...
      (.83597,4.6367E-06),(.854,4.762E-06),(.86952,4.8589E-06),...
      (.87784,4.911E-06),(.8822,4.9237E-06),(.88663,4.9332E-06),...
      (.89107,4.9392E-06),(.89551,4.9418E-06),(.89995,4.9407E-06),...
      (.90563,4.9279E-06),(.91451,4.8755E-06),(.92339,4.7849E-06),...
      (.93005,4.6898E-06),(.94115,4.4757E-06),(.95002,4.2506E-06),...
      (.96061,3.6106E-06),(.9706,2.8021E-06),(.98059,1.7824E-06),...
      (.99112,6.7472E-07),(.99778,1.7904E-07),(1.0,0.0)
      FUNCTION PSITH=(0.0,8.3132E-09),(.25854,7.6292E-09),...
      (.37049,7.6033E-09),(.44366,7.5786E-09),(.50615,7.5534E-09),...
      (.5461,7.5334E-09),(.64722,7.526E-09),(.69463,7.5808E-09),...
      (.73015,7.6866E-09),(.77863,8.0392E-09),(.812,8.5376E-09),...
      (.81999,8.6873E-09),(.83597,9.0214E-09),(.84956,9.5841E-09),...
      (.86231,1.0202E-08),(.87474,1.1102E-08),(.88663,1.1826E-08),...
      (.89551,1.2328E-08),(.90341,1.2835E-08),(.91007,1.3587E-08),...
      (.92117,1.4777E-08),(.93005,1.5618E-08),(.94115,1.6434E-08),...
      (.95002,1.6808E-08),(.95284,1.6884E-08),(.95395,1.6905E-08),...
      (.95506,1.6914E-08),(.95617,1.6911E-08),(.95728,1.6894E-08),...
      (.96061,1.6762E-08),(.96505,1.6324E-08),...
      (.9706,1.5245E-08),(.97504,1.3873E-08),(.98059,1.1394E-08),...
      (.98502,8.6903E-09),(.99112,5.1827E-09),(.99778,1.4947E-09),...
      (1.0,0.0)
      FUNCTION MEGATH=(0.0,1.5693E-11),(.25854,1.4063E-11),...
      (.37049,1.3887E-11),(.44366,1.3679E-11),(.50615,1.3485E-11),...
      (.58605,1.3032E-11),(.62059,1.2767E-11),(.67385,1.218E-11),...
      (.71239,1.1515E-11),(.75717,1.0429E-11),(.80401,8.6157E-12),...
      (.84956,6.7933E-12),(.86541,6.4125E-12),(.87474,6.5585E-12),...
      (.88663,7.2185E-12),(.90341,9.3944E-12),(.91007,1.1868E-11),...
      (.92117,1.7243E-11),(.93005,2.2643E-11),(.94115,3.0533E-11),...
      (.95002,3.7342E-11),(.96061,5.2119E-11),(.96505,5.7652E-11),...
      (.9706,6.2412E-11),(.97171,6.2956E-11),(.97282,6.3332E-11),...
```



```
                    (.97393,6.3524E-11),(.97504,6.3514E-11),(.97726,6.282E-11),...
                    (.98059,5.9793E-11),(.98502,5.1089E-11),(.99112,3.4986E-11),...
                    (.99778,1.122E-11),(1.0,0.0)
                    A1=NLFGEN(LAMDA,CTHETA)
                    A2=NLFGEN(CHITH,CTHETA)
                    A3=NLFGEN(PSITH,CTHETA)
                    A4=NLFGEN(MEGATH,CTHETA)
                    B1=A1*SQRT(T)
                    B2=A2*T
                    B3=A3*(T**1.5)
                    B4=A4*T*T
                    Z=B1+B2+B3+B4
                    THETA=CTHETA*(THETAO-THETAN)+THETAN
                    TIMER FINTIM=1.0,PRDEL=2.0E-02,OUTDEL=4.0E-02
                    PRTPLT Z
                    LABEL MOISTURE CONTENT PROFILE WITH TIME
                    PRINT THETA,A1,A2,B1,B2,B3,B4,Z
         END
         STOP

OUTPUT VARIABLE SEQUENCE
A4       B4       A3       B3       A2       B2       A1       B1       Z        THETA

 OUTPUTS     INPUTS     PARAMS   INTEGS + MEM BLKS   FORTRAN   DATA CDS
 14(500)    43(1400)   10(400)    0+   0=  0(300)    11(600)      54

         ENDJOB
```

used for Akuse clay). This program is slightly different from previous programs in this study in that it is not segmented into INITIAL, DYNAMIC and TERMINAL sections. This segmentation is not used in this program because the multiple run capability of the PARAMETER card which is used in this program to calculate water content profiles for the time periods specified does not require segmentation of the program.

Time is renamed CTHETA (Θ) which is equal to $(\theta-\theta_n)/(\theta_o-\theta_n)$ where θ is the moisture content for a particular λ, χ_w, ψ_w or ω_w; θ_o is the moisture content at $\lambda=0$, $\chi_w=0$, $\psi_w=0$ or $\omega_w=0$ and θ_n is the initial soil water content. The advantage with using the dimensionless water content in this program is that its minimum value is zero and maximum value is 1.0 and so simulation which must necessarily commence at zero proceeds without difficulties. On the other hand, if θ is used, the minimum value θ_n is not necessarily zero, thus requiring extrapolation so that computing starts at zero time.

In the INCON data card, two constants are specified, namely θ_o (THETAO) and θ_n (THETAN). The PARAMETER data card specifies four time periods T equal to 360s, 7200s, 19260s and 21600s for each of which the water content profile with depth is computed. The use of PARAMETER T = (360.0, 7200.0, 19260.0, 21600.0) will therefore cause the program to run first with T=360.0, second with T=7200.0, then with T=19260.0 and finally with T=21600.0.

Four tables are provided. The first, FUNCTION LAMBDA is a table of λ (Θ) with the first number in each bracket being the water content value and the second number, the corresponding λ value. FUNCTION CHITH is a table of χ_w (Θ). Again the first number in each parenthesis is the independent variable, water content and the second number is the dependent variable χ_w. The other two Tables are FUNCTION PSITH which is ψ_w (Θ) and FUNCTION MEGATH, ω_w (Θ). A non linear quadratic interpolation is used between data points provided by the four tables:

A1 = NLFGEN(LAMBDA,CTHETA) (4.207)

A2 = NLFGEN(CHITH,CTHETA) (4.208)

A3 = NLFGEN(PSITH,CTHETA) (4.209)

A4 = NLFGEN(MEGATH,CTHETA) (4.210)

Each of the terms on the righthand side of equation 3.68, that is $\lambda t^{1/2}$, $\chi_w t$, $\psi_w t^{3/2}$ and $\omega_w t^2$ is calculated as follows:

B1 = A1*SQRT(T) (4.211)

B2 = A2*T (4.212)

B3 = A3*(T**1.5) (4.213)

B4 = A4*T*T (4.214)

The depth z is then the sum of B1, B2, B3 and B4. A PRTPLT statement gives an output of a plot of Θ as a function of z. In addition THETA, A1, A2, B1, B2, B3, B4 and z are printed.

4.9.7 Description of CSMP program for simulating concentration of Cl^- profiles for various time periods for vertical infiltration of water and salt

The governing equation for simulation of concentration of Cl^-

profiles is equation 3.69. The program used for the simulation is given in figure 4.11 (see also Appendix J which provides the data for Akuse clay). This program, like the one presented in figure 4.10 for water content profile with time, is not segmented into INITIAL, DYNAMIC and TERMINAL sections.

Time is renamed CSEE, $C_2[=(c-c_n)/(c_o-c_n)]$ where c is the concentration of Cl^-, corresponding to a particular λ, χ_s, ψ_s or ω_s; c_o is the concentration of Cl^- at $\lambda=0$, $\chi_s=0$, $\psi_s=0$ and $\omega_s=0$; and c_n is the initial concentration of Cl^- in the soil.

In the data card INCON, two constants, namely c_o (SEEO) and c_n (SEEN) are specified. Four time periods viz: 360s, 7200s, 19260s, and 21600s are specified in the PARAMETER card. Like the program in figure 4.10, the use of PARAMETER T = (360.0, 7200.0, 19260.0, 21600.0) enable the program to run first with T = 360.0, second with T = 7200.0, then with T = 19260.0 and finally with T = 21600.0.

The following four tables for $\lambda(C_2)$, $\chi_s(C_2)$, $\psi_s(C_2)$ and $\omega_s(C_2)$ respectively are provided: FUNCTION CLAMDA, FUNCTION CHIS, FUNCTION PSIS and FUNCTION OMEGAS. In these tables, the independent variable C_2 is listed first in each of the parentheses. The dependent variable is the second value in the bracket.

A Lagrange quadratic interpolation is used between the data points given in the four tables:

```
A1  =  NLFGEN(CLAMDA, CSEE)
A2  =  NLFGEN(CHIS, CSEE)
A3  =  NLFGEN(PSIS, CSEE)
```

FIGURE 4.11

CSMP listing for simulating concentration of Cl^- profiles for various time periods for vertical infiltration of water and salt (Brookston clay).

```
                  ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

     TITLE CHLORIDE CONCENTRATION PROFILES WITH TIME (BROOKSTON CLAY)
     *     UNITS
     *     KG=KILOGRAMS
     *     M=METERS
     *     KEQ=KILO-EQUIVALENTS
     *     S=SECONDS
     *     GLOSSARY OF SYMBOLS
     *     CSEE=DIMENSIONLESS CONCENTRATION
     *     SEEO=CONCENTRATION OF CHLORIDE AT LAMBDA EQUALS ZERO , CHI FOR
     *     SALT EQUALS ZERO, PSI FOR SALT EQUALS ZERO, AND OMEGA FOR SALT
     *     EQUALS ZERO
     *     SEEN=INITIAL CONCENTRATION OF CHLORIDE IN THE MOIST SOIL
     *     CLAMDA=TABLE OF LAMBDA AND CORRESPONDING CONCENTRATION VALUES
     *     CHIS=TABLE OF CHI FOR SALT AND CORRESPONDING CONCENTRATION VALUES
     *     PSIS=TABLE OF PSI FOR SALT AND CORRESPONDING CONCENTRATION VALUES
     *     OMEGAS=TABLE OF OMEGA FOR SALT AND CORRESPONDING CONCENTRATION
     *     VALUES
     *     T=TIME
     *     SEE=CONCENTRATION OF CHLORIDE IN SOLUTION
      RENAME TIME=CSEE
           INCON SEEO=.97,SEEN=.00018
           PARAMETER T=(360.0,7200.0,19260.0,21600.0)
           FUNCTION CLAMDA=(0.0,1.82E-03),(6.3105E-03,1.8018E-03),...
           (8.9914E-03,1.7654E-03),(1.2291E-02,1.729E-03),...
           (1.6553E-02,1.6926E-03),(2.3994E-02,1.6562E-03),...
           (3.776E-02,1.6198E-03),(5.9345E-02,1.5834E-03),...
           (8.9006E-02,1.547E-03),(.10994,1.5288E-03),...
           (.17799,1.4924E-03),(.32977,1.456E-03),(.55868,1.4196E-03),...
           (.70304,1.3832E-03),(.79258,1.3468E-03),(.83762,1.3104E-03),...
           (.87462,1.274E-03),(.91266,1.2194E-03),(.9288,1.183E-03),...
           (.94194,1.1466E-03),(.96041,1.092E-03),(.97166,1.0374E-03),...
           (.98115,9.828E-04),(.98866,9.1E-04),(.99392,8.554E-04),...
           (.99737,8.19E-04),(.99921,7.644E-04),(.9994,5.824E-04),...
           (.99961,3.822E-04),(.99981,1.82E-04),(.99991,9.1E-05),...
           (1.0,0.0)
           FUNCTION CHIS=(0.0,2.0859E-06),(7.6509E-03,2.39E-06),...
           (8.9914E-03,2.4179E-06),(1.2291E-02,2.4659E-06),...
           (1.6553E-02,2.5058E-06),(2.3994E-02,2.5585E-06),...
           (3.776E-02,2.565E-06),(5.9345E-02,2.585E-06),...
           (8.9006E-02,2.6003E-06),(.13809,2.6108E-06),...
           (.17799,2.6141E-06),(.23594,2.616E-06),(.32977,2.6153E-06),...
           (.55868,2.6071E-06),(.70304,2.5902E-06),(.79258,2.5673E-06),...
           (.83762,2.5395E-06),(.87462,2.5072E-06),(.90328,2.4704E-06),...
           (.9288,2.4082E-06),(.95507,2.3128E-06),(.96791,2.2309E-06),...
           (.97917,2.141E-06),(.9849,2.044E-06),(.99047,1.9412E-06),...
           (.99392,1.869E-06),(.99737,1.7937E-06),(.99921,1.6755E-06),...
           (.99931,1.4777E-06),(.9994,1.2795E-06),(.99951,1.0411E-06),...
           (.99961,8.4204E-07),(.9997,6.4246E-07),(.9998,4.0227E-07),...
           (.99991,2.0146E-07),(1.0,0.0)
           FUNCTION PSIS=(0.0,3.6835E-09),(7.6509E-03,5.1961E-09),...
           (1.0414E-02,5.2801E-09),(1.4168E-02,5.3547E-09),...
           (2.3994E-02,5.4508E-09),(3.776E-02,5.5038E-09),...
           (7.1787E-02,5.5689E-09),(.10994,5.6059E-09),...
           (.17799,5.6406E-09),(.32977,5.675E-09),(.55868,5.7039E-09),...
           (.70304,5.7224E-09),(.74995,5.7286E-09),(.79258,5.7322E-09),...
           (.8151,5.7341E-09),(.83762,5.7341E-09),(.85773,5.7315E-09),...
           (.89151,5.719E-09),(.91266,5.6959E-09),(.9288,5.6627E-09),...
           (.94194,5.6191E-09),(.95507,5.5617E-09),(.96791,5.4472E-09),...
           (.97917,5.2991E-09),(.98303,5.1814E-09),(.98866,4.9816E-09),...
           (.99219,4.8299E-09),(.99565,4.6616E-09),(.9991,4.4732E-09),...
```

```
                  (.9993,3.776E-09),(.9994,3.2756E-09),(.9995,2.6719E-09),...
                  (.9996,2.1656E-09),(.9997,1.6562E-09),(.9998,1.0401E-09),...
                  (.99991,5.2231E-10),(.99994,3.1394E-10),(1.0,0.0)
                  FUNCTION OMEGAS=(0.0,6.8682E-12),(6.3105E-03,9.3284E-12),...
                  (8.9914E-03,9.3404E-12),(1.2291E-02,9.3874E-12),...
                  (1.6553E-02,9.4412E-12),(2.8686E-02,9.5213E-12),...
                  (4.7968E-02,9.5676E-12),(7.1787E-02,9.5988E-12),...
                  (.10994,9.6175E-12),(.17799,9.6286E-12),(.32977,9.6547E-12),...
                  (.55868,9.6975E-12),(.70304,9.7423E-12),(.79258,9.7923E-12),...
                  (.83762,9.8475E-12),(.87462,9.9049E-12),(.90328,9.9605E-12),...
                  (.92205,1.0011E-11),(.93537,1.0055E-11),(.94851,1.0085E-11),...
                  (.95507,1.0091E-11),(.96416,1.0083E-11),(.97166,1.0049E-11),...
                  (.97917,9.9749E-12),(.9849,9.7977E-12),(.99047,9.5335E-12),...
                  (.99392,9.2948E-12),(.99737,8.9942E-12),(.99919,8.6173E-12),...
                  (.99925,8.0444E-12),(.99931,7.469E-12),(.9994,6.5026E-12),...
                  (.99951,5.3291E-12),(.99961,4.3377E-12),(.9997,3.3323E-12),...
                  (.99981,2.1048E-12),(.99991,1.0621E-12),(.99994,6.3965E-13),...
                  (1.0,0.0)
                  A1=NLFGEN(CLAMDA,CSEE)
                  A2=NLFGEN(CHIS,CSEE)
                  A3=NLFGEN(PSIS,CSEE)
                  A4=NLFGEN(OMEGAS,CSEE)
                  B1=A1*SQRT(T)
                  B2=A2*T
                  B3=A3*(T**1.5)
                  B4=A4*T*T
                  Z=B1+B2+B3+B4
                  SEE=CSEE*(SEEO-SEEN)+SEEN
                  TIMER FINTIM=1.0,PRDEL=2.0E-02,OUTDEL=4.0E-02
                  PRTPLT Z
                  LABEL CONCENTRATION PROFILE WITH TIME
                  PRINT SEE,A1,A2,B1,B2,B3,B4,Z
          END
          STOP

OUTPUT VARIABLE SEQUENCE
A4      B4      A3      B3      A2      B2      A1      B1      Z       SEE

 OUTPUTS     INPUTS     PARAMS   INTEGS + MEM BLKS   FORTRAN   DATA CDS
 14(500)    43(1400)   10(400)    0+   0=  0(300)    11(600)      64

          ENDJOB
```

```
A4 = NLFGEN(OMEGAS, CSEE)
```

The terms $\lambda t^{1/2}$, $\chi_s t$, $\psi_s t^{3/2}$ and $\omega_s t^2$ in equation 3.69 are calculated respectively through the statements:

```
B1 = A1*SQRT(T)
B2 = A2*T
B3 = A3*(T**1.5)
B4 = A4*T*T
```

The sum of B1, B2, B3 and B4 gives the depth z. A PRTPLT statement gives a plot of C_2 as a function of z and this plotting is labelled concentration profile with time. Print output for CSEE, A1, A2, B1, B2, B3, B4 and z are also obtained.

CHAPTER 5

RESULTS AND DISCUSSION

5.1 Relative Adsorption Rates and Adsorption Isotherms

Two models are usually used to describe the adsorption and exchange phenomena in the convective-dispersive hydrodynamic equation. One of the models represents an equilibrium between the concentration of a chemical in solution and that on the adsorbed phase (Bower _et al_., 1957; Lapidus and Amundson, 1952; Kay and Elrick, 1967; Lindstrom and Boersma, 1970; Lai and Jurinak, 1971). The other models the rate of approach to equilibrium (Bower _et al_., 1957; Lapidus and Amundson, 1952; Lindstrom _et al_., 1971). In the horizontal infiltration experiments considered in this study it was necessary to ascertain which of these two models best describes the adsorption or exchange phenomenon. The relationship between the keq. K^+ adsorbed per kg. soil plotted against various equilibration times (figure 5.1) indicates that equilibrium was established between the adsorbed and solution phases of potassium in less than 600 s. One would expect progressively increasing quantities of K^+ adsorbed with increasing equilibration time periods if a slow kinetic type of reaction pertains in the adsorption process of K^+ in these soils. Figure 5.1, therefore, appears to indicate an establishment of an almost instantaneous equilibrium and thus justifies the use of an equilibrium type of model to describe the adsorption term in the hydrodynamic equation for the movement of reactive solutes in the soils used in this study.

The adsorption isotherms for Akuse and Brookston clays plotted as kiloequivalent K^+ adsorbed per kilogram soil against equilibrium

FIGURE 5.1.

Quantity of K^+ adsorbed at different time periods.

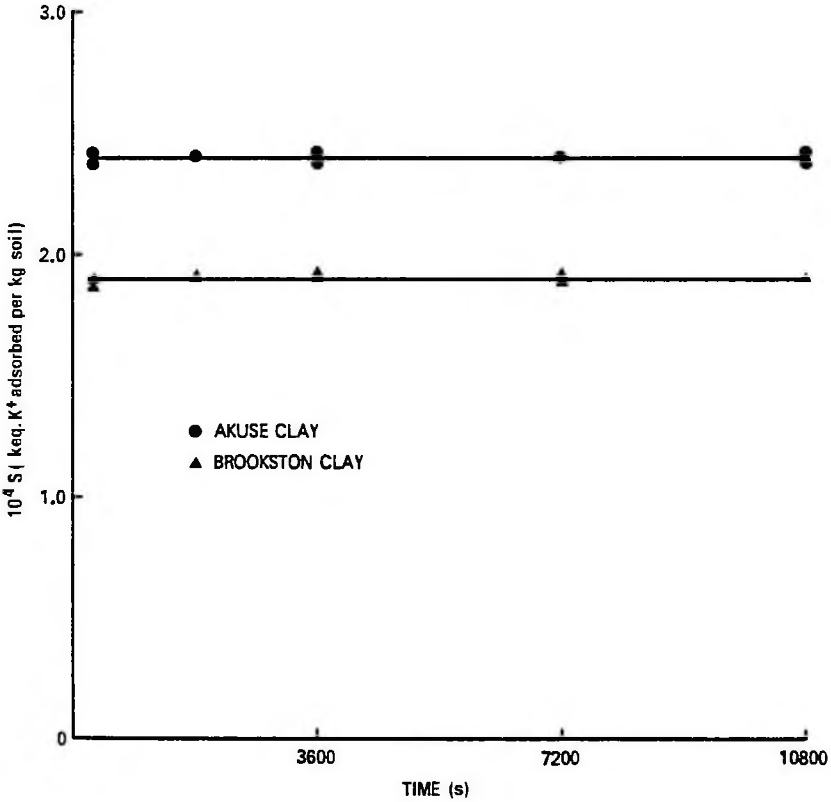

3.0
2.0
1.0
0
10^4 S (keq. K^+ adsorbed per kg soil)
3600
7200
10800
TIME (s)
● AKUSE CLAY
▲ BROOKSTON CLAY

Figure 5.1

concentration (in kiloequivalent K^+ per cubic meters of solution) are given in figures 5.2 and 5.3. It is observed that over the concentration range of 1.0×10^{-4} to 1.0 keq/m^3, the adsorption isotherms of the two soils do not obey the Freundlich's equation of the form $S_{ads.} = kc^n$, where k and n are constants. In our horizontal infiltration experiments where concentration in the soil column can vary from 1.0 keq/m^3 at the inlet to zero at the wetting front, it was necessary to fit equations to the adsorption isotherms. The isotherms were fitted with polynomial equation of the logarithmic form to obtain

$$S = 10^{(-0.1205\log^{2}c+0.1292\log c-3.6124)} \text{ for Akuse clay}$$

and $$S = 10^{(-0.1029\log^{2}c+0.1268\log c-3.7163)} \text{ for Brookston clay.}$$

These equations were used to calculate the concentration of K^+ in solution for the horizontal infiltration as outlined in Chapter 4. It has to be mentioned that the coefficients in these two equations for the adsorption isotherm will be different if the units are changed, thus if the isotherms are plotted in milliequivalent of K^+ adsorbed per gram soil versus milliequivalents K^+ in solution per litre, the equations for Akuse clay and Brookston clay become, respectively,

$$S = 10^{(-0.1205\log^{2}c+0.8520\log c-2.084)}$$

and $$S = 10^{(-0.1029\log^{2}c+0.7444\log c-2.0231)}$$

In the computation of the dispersion coefficient D_s for K^+ using

FIGURE 5.2.

K^+ adsorption isotherm on soil fractions of Ca^{2+}-saturated Akuse clay.

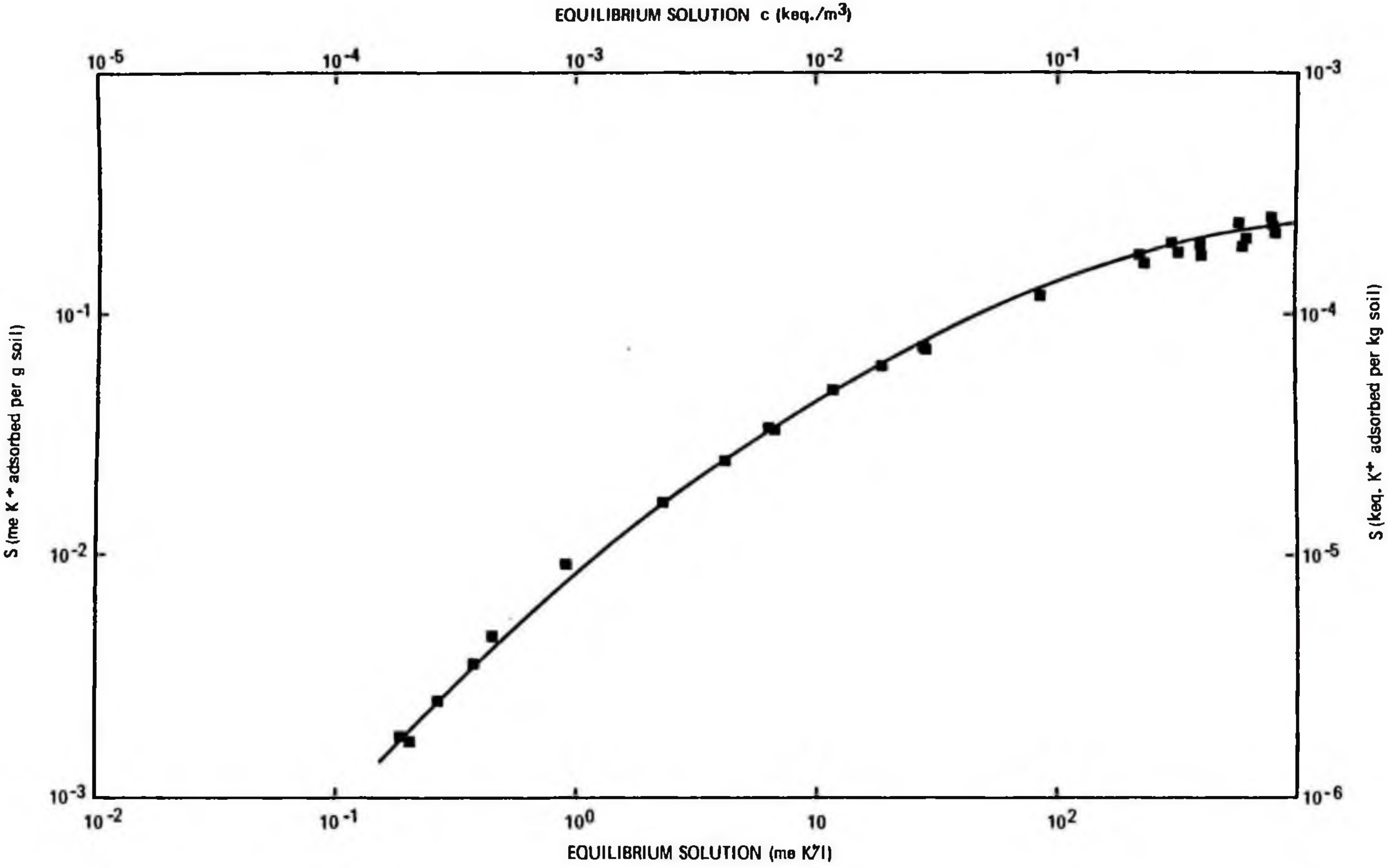

EQUILIBRIUM SOLUTION c (keq./m^3)
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
S (keq. K$^+$ adsorbed per kg soil)
S (me K$^+$ adsorbed per g soil)
10^{-1}
10^{-2}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10
10^{2}
EQUILIBRIUM SOLUTION (me K$^+$/l)

Figure 5.2

FIGURE 5.3.

K^+ adsorption isotherm on soil fraction of Ca^{2+}-saturated Brookston clay.

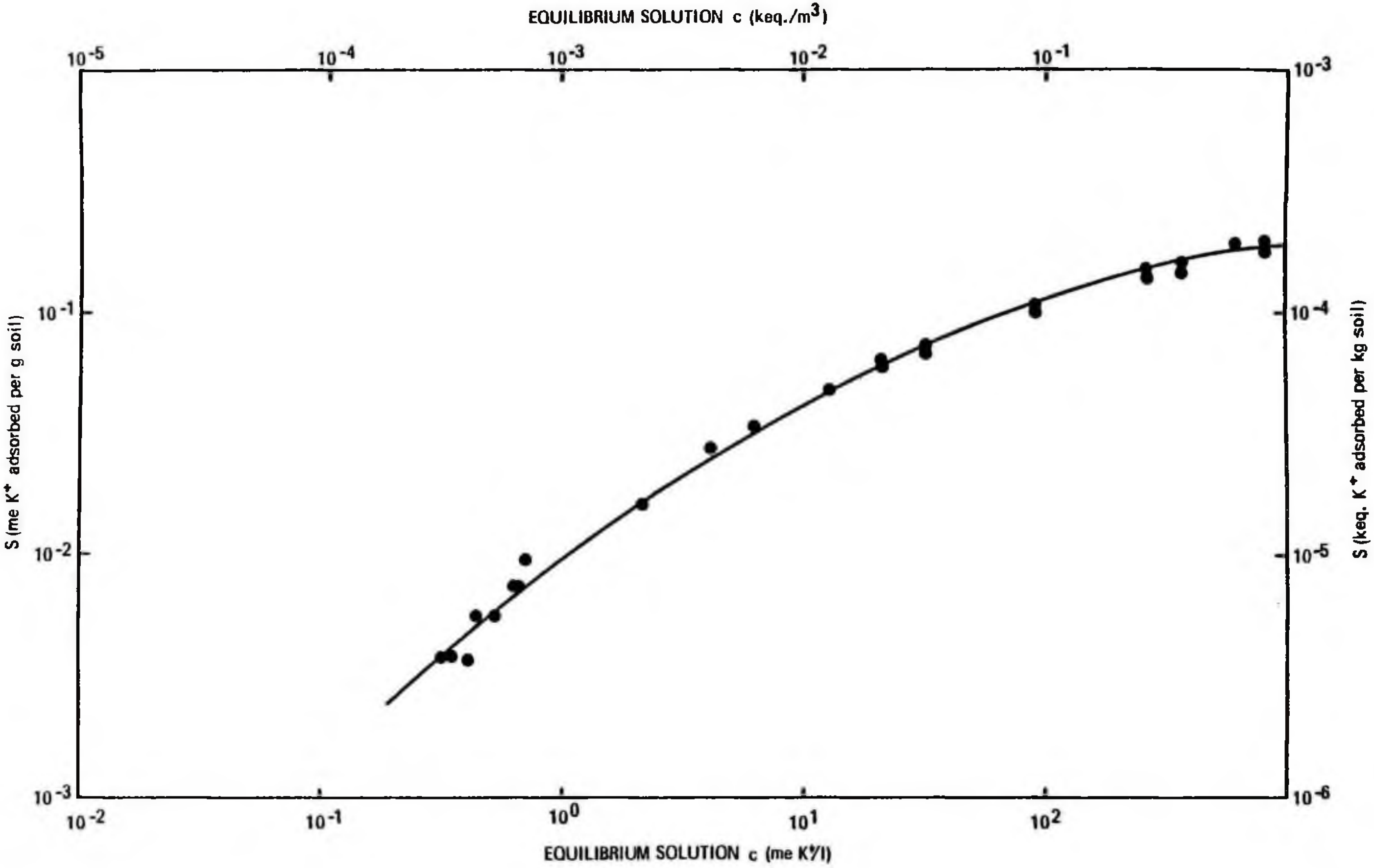

EQUILIBRIUM SOLUTION c (keq./m^3)
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
S (keq. K$^+$ adsorbed per kg soil)
S (me K$^+$ adsorbed per g soil)
10^{-1}
10^{-2}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
EQUILIBRIUM SOLUTION c (me K$^+$/l)

Figure 5.3

a computer program written in system 360 CSMP data points from figures 5.2 and 5.3 provided FUNCTION ADSISO which was interpolated, and derivative performed to obtain dS/dλ used in the computation.

Lastly, it must be mentioned that, in a preliminary experiment, it was observed that no Cl^- was adsorbed when the same concentration range of $1.0x10^{-4}$ to 1.0 keq/m^3 KCl was equilibrated with known weights of the two soils used in this study. The low concentration of chloride measured for lambda values between zero and $1.1x10^{-3}$ $mS^{-1/2}$ cannot therefore be ascribed to chloride adsorption by amorphous aluminum and iron oxides in these soils.

5.2 Horizontal Infiltration with KCl solution

Figures 5.4a and 5.4b present the bulk density profiles in the soil columns used for the horizontal infiltration experiments for Akuse clay and Brookston clay, respectively. The low mean bulk densities of $1.03x10^3$ kg/m^3 and $1.07x10^3$ kg/m^3 for Akuse clay and Brookston clay, respectively, are the bulk densities which could be reproduced fairly well in replicate infiltration runs. Any attempt to pack these moist soils (initial moisture content of 0.10 and 0.12 for Akuse clay and Brookston clay, respectively) to higher bulk densities resulted in uneven bulk density distribution in the columns which could not be reproduced for subsequent infiltration runs.

Figures 5.5 and 5.6 present the θ, c_{Cl^-}, and c_{K^+} profiles of the horizontal experiments listed in Table 5.1. The smoothed curves of

TABLE 5.1. Experimental conditions imposed during horizontal and vertical infiltration experiments

Soil	Type of Infiltration	Initial volumetric water Content θ_n	Initial Cl^- Concentration keq/m^3	Initial K^+ Concentration keq/m^3	Mean Bulk Density in Soil Column $10^{-3}\rho$ kg/m^3	Measured Sorptivity 10^3 SORP. $m/s^{1/2}$	Time t s
Akuse Clay	Horizontal	0.099	0.00023	0.0	1.021	}1.749	2,615
		0.105	0.00024	0.0	1.030		3,745
		0.107	0.00022	0.0	1.024		5,558
		0.110	0.00025	0.0	1.046		9,330
	Vertical	0.101	0.0003	0.0	1.041	-	7,200
Brookston Clay	Horizontal	0.124	0.005	0.0	1.06	}0.6518	3,600
		0.118	0.005	0.0	1.07		7,200
		0.122	0.005	0.0	1.07		14,400
		0.120	0.005	0.0	1.06		21,600
	Vertical	0.124	0.0002	0.0	1.08		19,260
Akuse Clay (dry soil initially)	Horizontal	0.053	0.001	0.0	1.266	}0.7182	3,600
		0.054	0.002	0.0	1.271		5,400
		0.054	0.002	0.0	1.271		10,800
		0.050	0.002	0.0	1.266		14,400

FIGURE 5.4.

(a) Bulk density distribution in soil columns used for the horizontal infiltration (Akuse clay).

(b) Bulk density distribution in soil columns used for the horizontal infiltration (Brookston clay).

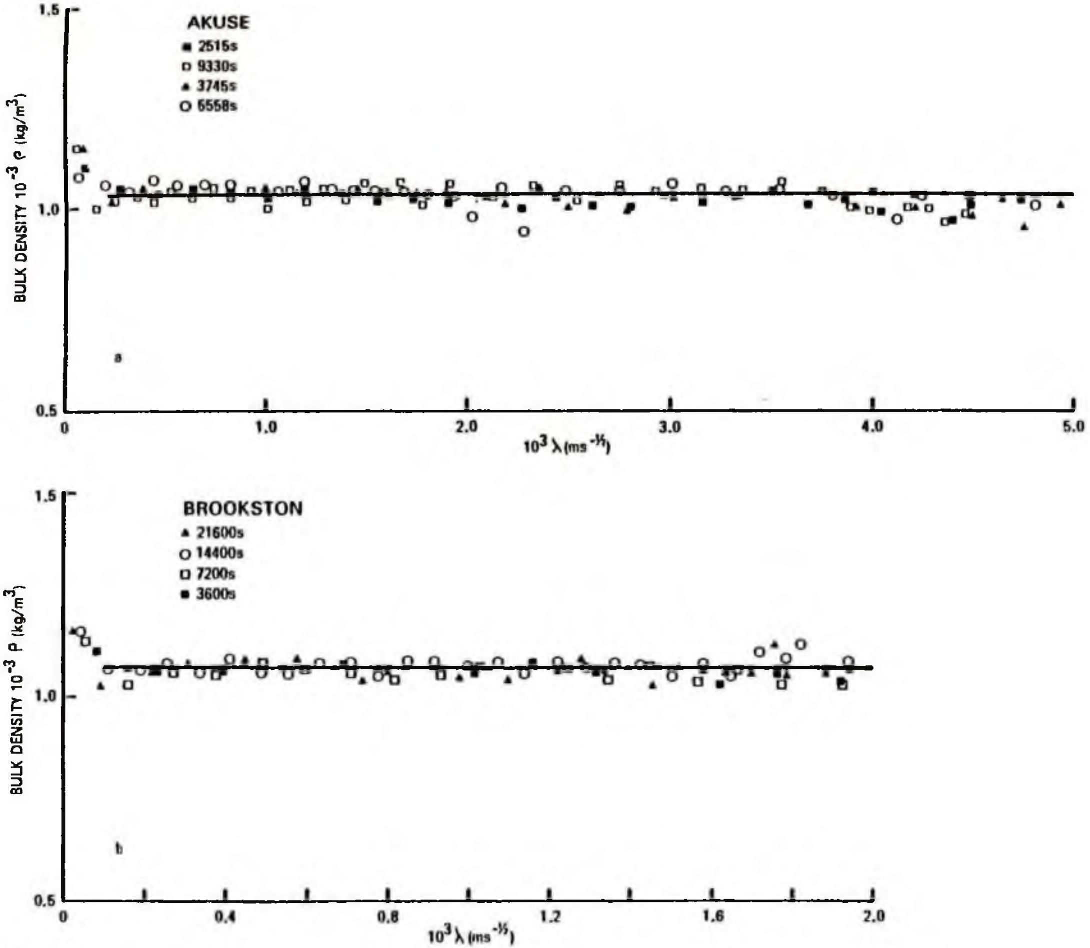

AKUSE
■ 2515s
□ 9330s
▲ 3745s
○ 6558s
BULK DENSITY 10^{-3} ρ (kg/m^3)
1.5
1.0
0.5
a
0
1.0
2.0
3.0
4.0
5.0
10^3 λ (ms$^{-½}$)
BROOKSTON
▲ 21600s
○ 14400s
□ 7200s
■ 3600s
BULK DENSITY 10^{-3} ρ (kg/m^3)
1.5
1.0
0.5
b
0
0.4
0.8
1.2
1.6
2.0
10^3 λ (ms$^{-½}$)

Figure 5.4

best fit were drawn by eye. The first observation from figures 5.5 and 5.6 is that as was found by Smiles et al. (1978), Smiles and Philip (1978) and also by Elrick et al. (1979) (under review), the water content, chloride content and potassium content profiles all preserve similarity in terms of $\lambda = xt^{-1/2}$, reasonably well. Variability in packing the soil columns (figure 5.4a and 5.4b), problems of air entrapment and losses of small amounts of solution during division of soil sample from each section for Cl^- and K^+ determinations, likely account for the variability in the data. Both the cumulative volume of solution as well as the distance to the wetting front as functions of $t^{1/2}$ for each experimental run gave excellent straight lines which passed through the origin. However, due to the experimental difficulties listed above, the slopes of these lines differed very slightly from one column to another. Generally, it is accepted that the water flow equation is valid, so we use the uniqueness of $\theta(\lambda)$ as a guide to provide a basis for examination of the $c_{Cl^-}(\lambda)$ and $c_{K^+}(\lambda)$ relationships in figures 5.5 and 5.6 and conclude that the $c_{Cl^-}(\lambda)$ and $c_{K^+}(\lambda)$ curves are unique and therefore the assumption that D_s be considered only as a function of θ is justified. Justification of this assumption is also confirmed by the work of Smiles et al. (1978), Smiles and Philip (1978) and Elrick et al. (1979).

We next observe that the "salt front" for Cl^- lags behind the infiltration front (cf. figures 5.5a and b and also figures 5.6a and b). This effect, due to "piston flow", is observed because if there is hydrodynamic dispersion and the initial water content of the soil >0, the original water and the encroaching solution mix across the solute penetration depth resulting in the development of a transition zone in which the concentration varies from c_n to c_0. The salt front or transition zone usually lags behind the infiltration front because at least some of the antecedent soil water is pushed ahead of the salt front. This result is consistent with the previous studies of Warrick *et al*. (1971); Kirda *et al*. (1973, 1974); Ghuman *et al*. (1975); Smiles *et al*. (1978) and Smiles and Philip (1978). Shalhevet and Reiniger (1964) and Terkeltoub and Babcock (1971) also used this principle of "piston flow" to formulate leaching strategies.

The notional plane $\lambda = \lambda'$, about which chloride dispersion occurs may be defined by the material balance equation

$$\int_0^{\lambda} (c_o - c)\, d\lambda = \int_{\lambda'}^{\infty} (c - c_n)\, d\lambda \tag{5.1}$$

Similarly, the plane $\lambda = \lambda^*$ defining the plane of separation, if the water initially in the soil column were perfectly displaced by the encroaching solution, is defined by the material balance equation

$$\lambda^* \, \theta(\lambda^*) = \int_{\theta_n}^{\theta(\lambda^*)} \lambda d\theta \tag{5.2}$$

These two planes are identified in the $c_{Cl^-}(\lambda)$ and $\theta(\lambda)$ plots (figures 5.5a, b and 5.6a, b). One expects these two planes to coincide exactly ($\lambda'=\lambda^*$) if all the initial water content is swept entirely ahead of the salt front, that is if there is perfect piston flow without any mixing or transition zone. For the soils under consideration in this study, these two planes for λ' and λ^* do not correspond exactly as was reported by Smiles and Philip (1978) for the sand/kaolin mixture. The possible explanation to this is partly due to mixing which is reflected in a dispersed salt front compared with the sharp, abrupt water front (cf. figures 5.5a and 5.5b and also 5.6a and 5.6b) and also partly due to anion exclusion, and "immobile" water fraction in dead end pores in these aggregated clays whose aggregates are still visible even after grinding and sieving to pass through 0.25 mm sieves (Fatt *et al*., 1960; Coats and Smith, 1964; Philip, 1968; van Genuchten and Wierenga, 1976; Gaudet *et al*., 1977).

Also, defining mean pore water velocity u in terms of the Darcy flux v and volumetric water content θ as:

$$u = v/\theta \qquad (5.3)$$

substitution of $v = -D\, d\theta/dx$, transformation with the Boltzmann transform $\lambda = xt^{-1/2}$ and further substitution of $-D\frac{d\theta}{d\lambda} = \frac{1}{2}\int_{\theta_n}^{\theta}\lambda d\theta$ yields

$$u = \frac{t^{-1/2}}{2\theta}\int_{\theta_n}^{\theta}\lambda d\theta \qquad (5.4)$$

FIGURE 5.5.

(a) Experimental moisture content data points $\theta(\lambda)$,

(b) experimental solution concentration data points for Cl^- $c_{Cl^-}(\lambda)$, and

(c) experimental solution concentration data points for K^+ $c_{K^+}(\lambda)$.

The vertical broken lines identify λ^* and λ' planes calculated as described in the text (Akuse clay initially moist).

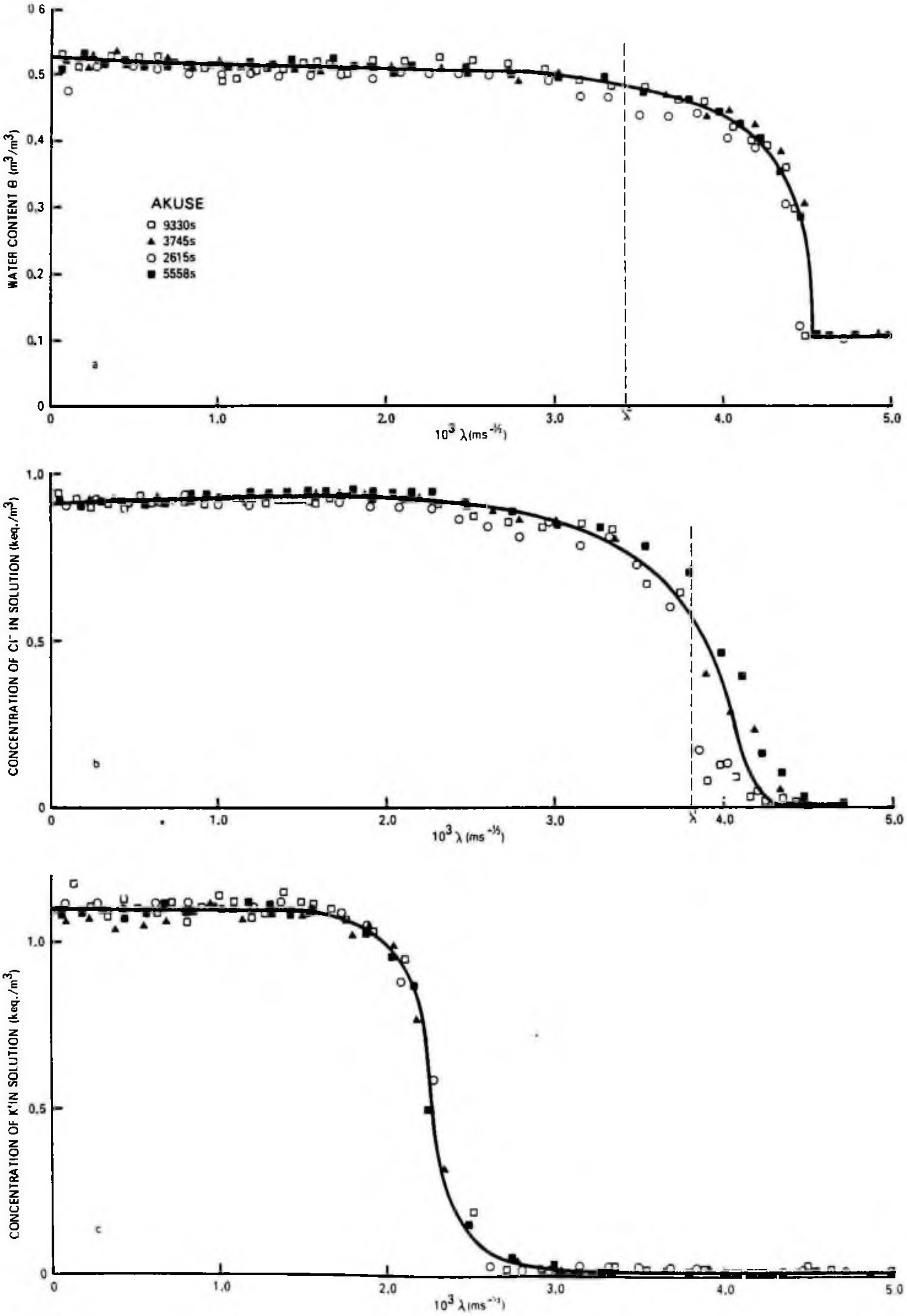

WATER CONTENT θ (m^3/m^3)
0.6
0.5
0.4
0.3
0.2
0.1
0
AKUSE
□ 9330s
▲ 3745s
○ 2615s
■ 5558s
a
1.0
2.0
3.0
λ'
4.0
5.0
10^3 λ (ms$^{-½}$)
CONCENTRATION OF Cl$^-$ IN SOLUTION (keq./m^3)
1.0
0.5
0
b
λ'
10^3 λ (ms$^{-½}$)
CONCENTRATION OF K$^+$IN SOLUTION (keq./m^3)
c
10^3 λ (ms$^{-½}$)

Figure 5.5

FIGURE 5.6.

(a) Experimental moisture content data points $\theta(\lambda)$,

(b) experimental solution concentration data points for Cl^- $c_{Cl^-}(\lambda)$, and

(c) solution concentration data points for K^+ $c_{K^+}(\lambda)$.

The vertical broken lines identify λ^* and λ' planes calculated as described in the text (Brookston clay).

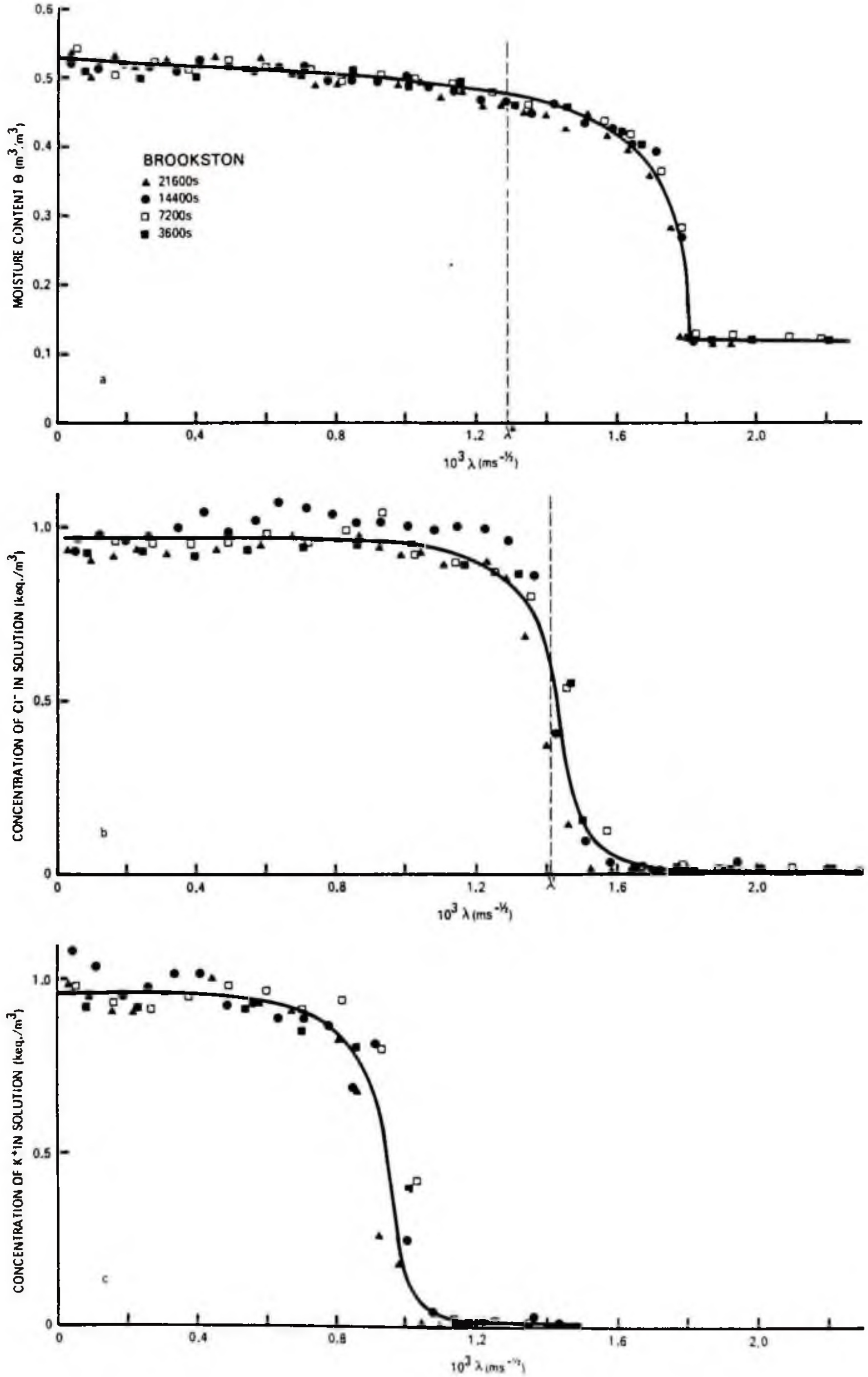

MOISTURE CONTENT θ (m^3/m^3)
0
0.1
0.2
0.3
0.4
0.5
0.6
BROOKSTON
▲ 21600s
● 14400s
□ 7200s
■ 3600s
a
0
0.4
0.8
1.2
λ*
1.6
2.0
10^3 λ (ms$^{-½}$)
CONCENTRATION OF Cl$^-$ IN SOLUTION (keq./m^3)
0
0.5
1.0
b
0
0.4
0.8
1.2
λ*
1.6
2.0
10^3 λ (ms$^{-½}$)
CONCENTRATION OF K$^+$ IN SOLUTION (keq./m^3)
0
0.5
1.0
c
0
0.4
0.8
1.2
1.6
2.0
10^3 λ (ms$^{-½}$)

Figure 5.6

If we further define a reduced mean pore water velocity u* as

$u^* = ut^{1/2}$, equation 5.4 becomes

$$u^*(\lambda) = \frac{1}{2\theta}\int_{\theta_n}^{\theta} \lambda d\theta \qquad (5.5)$$

Computation of the reduced mean pore water velocity from figures 5.5a and 5.6a reveals that the reduced mean pore water velocity tends to increase very slightly to a maximum at λ* (figures 5.7a and 5.7b). The maximum reduced mean pore water velocity appears to coincide with the region where the dispersion coefficient D_s is minimum. This latter finding is unexpected and presumably relates to our initial assumption of non-dependence of D_s on the pore water velocity.

The concentration of Cl^- profile for Akuse clay (figure 5.5b) extrapolated to λ=0, indicates that this concentration is about 8% lower than the inlet concentration of 1.0 keq/m^3. This is attributed to chloride exclusion which is discussed in the next section. The concentration profile of K^+ (figure 5.5c) for Akuse, extrapolated to λ=0, on the other hand, shows an increase of about 9%. It was expected, as observed in figures 5.6b and 5.6c, that both K^+ and Cl^- concentrations at λ=0 will be equal, in order to preserve electroneutrality. This difference, however, cannot be explained.

As a result of adsorption, the potassium content profiles for both Akuse clay and Brookston clay (figures 5.5c and 5.6c) lag greatly

FIGURE 5.7.

(a) Reduced mean pore water velocity versus λ for Akuse clay.

(b) Reduced mean pore water velocity versus λ for Brookston clay.

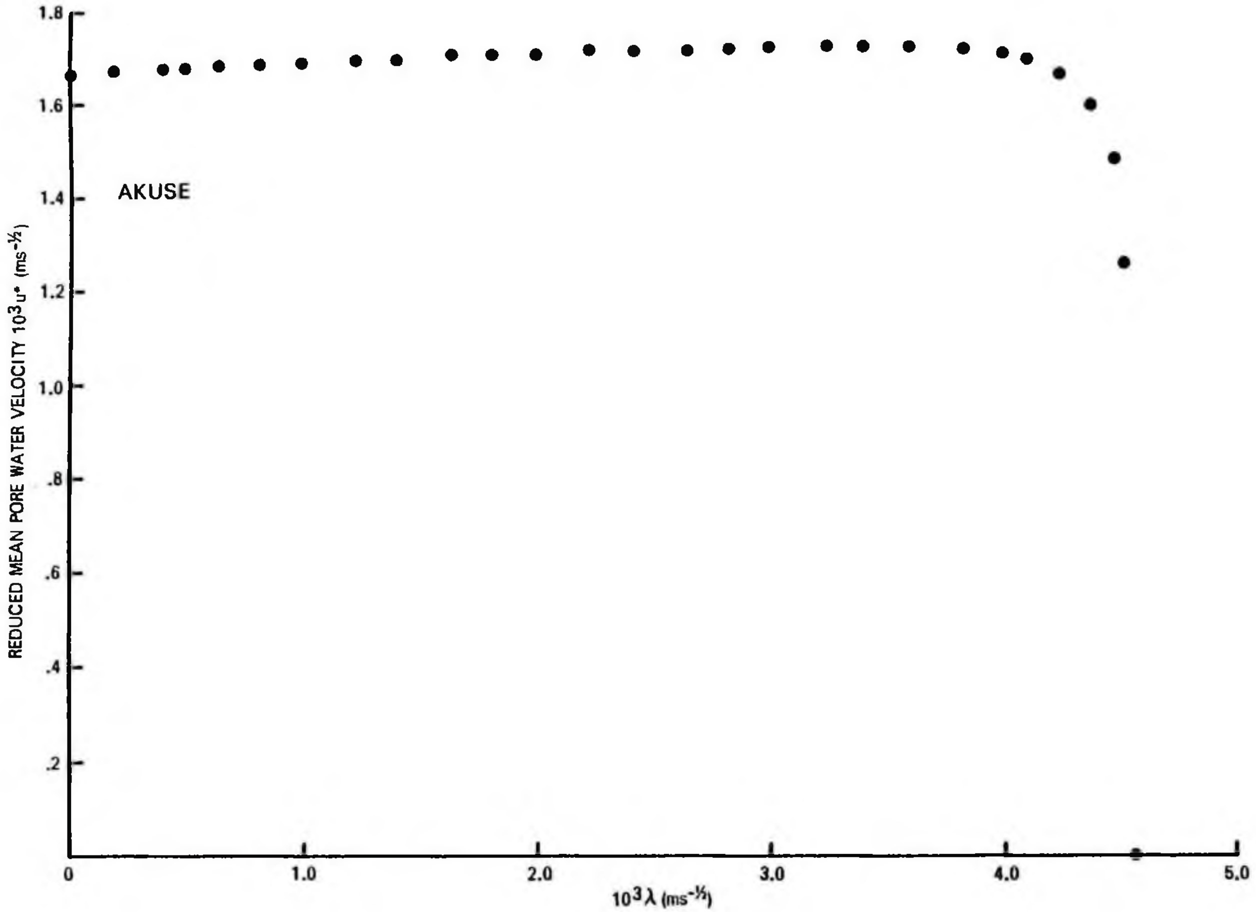

REDUCED MEAN PORE WATER VELOCITY $10^3 u^*$ (ms$^{-½}$)
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
AKUSE
0
1.0
2.0
3.0
4.0
5.0
$10^3 \lambda$ (ms$^{-½}$)

Figure 5.7a

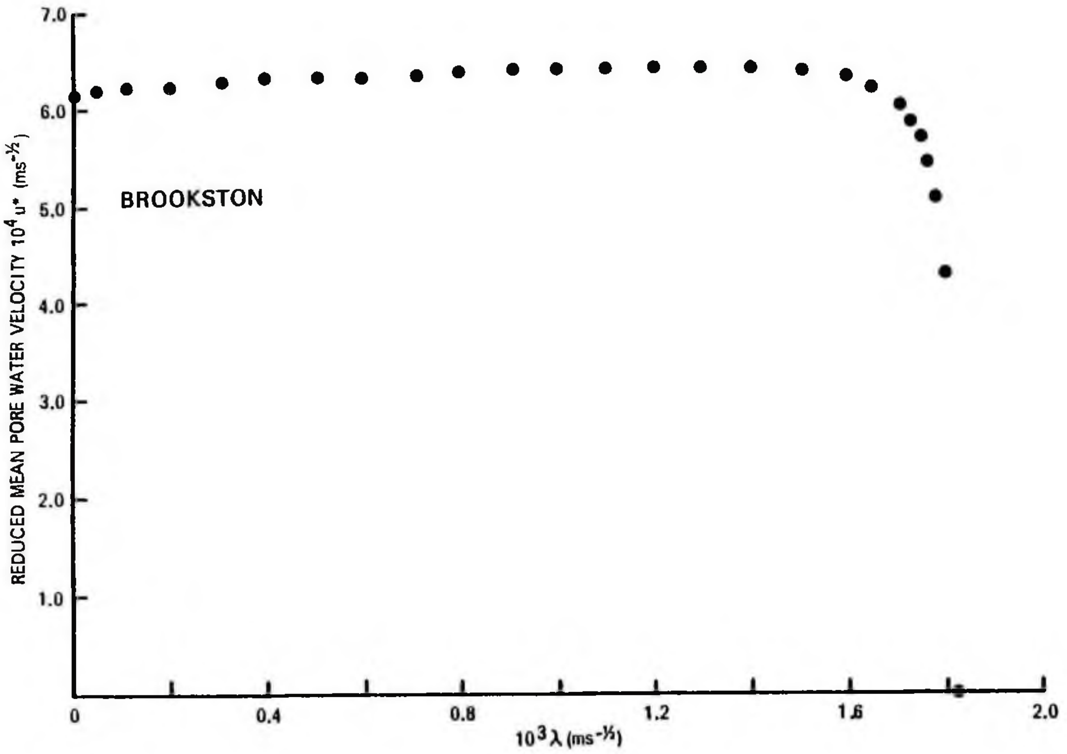

REDUCED MEAN PORE WATER VELOCITY $10^4 u^*$ ($ms^{-½}$)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
BROOKSTON
0
0.4
0.8
1.2
1.6
2.0
$10^3 \lambda$ ($ms^{-½}$)

Figure 5.7b

behind both the 'chloride front' and the infiltration front. At $\lambda=3.0\text{x}10^{-3}$ $ms^{-1/2}$, there is practically no K^+ in solution for Akuse clay even though the infiltration front is at $\lambda=4.56\text{x}10^{-3}$. Similarly, for Brookston clay, at $\lambda=1.17\text{x}10^{-3}$ $ms^{-1/2}$ there was no measurable amount of K^+ in solution even though the infiltration front is at $\lambda=1.82\text{x}10^{-3}$. Comparison of figures 5.5b and 5.5c appear to indicate a sharper 'concentration front' for K^+ than for Cl^- in the case of Akuse clay whilst both concentration front for K^+ and Cl^- for Brookston are not distinguishably different.

5.3 Effect of salt exclusion in the infiltration experiments

The set of horizontal infiltration data which show the effects of salt sieving were obtained with infiltration of KCl solution into air dried Akuse clay at volumetric water content of 0.05 m^3/m^3 and would be referred to as Akuse (dry) to distinguish it from the results in the previous section for Akuse clay initially packed moist into the columns. To facilitate comparison, especially, of the concentration of Cl^- profile, data for air dried Caledon sandy loam (66.0% sand, 30.5% silt and 3.5% clay) are also presented. The bulk density profile (figure 5.8a) for the soil columns initially packed with air dried Akuse clay, shows a fairly uniform packing with slightly higher bulk densities at the inlet end than the mean bulk density of $1.26\text{x}10^3$ kg/m^3. Also, because packing was done with air dried soil, reproducible packing was obtained with higher bulk densities in these experiments than those reported for the infiltration runs conducted with moist Akuse clay. The Caledon sandy loam was packed to a mean bulk density of $1.57\text{x}10^3$ kg/m^3 (figure 5.8b). The inlet end, however, showed higher bulk density

FIGURE 5.8.

Bulk density profile for soil columns used in the horizontal infiltration experiment for:

(a) Air-dried Akuse clay $\theta = 0.05$

(b) Air-dried Caledon fine sandy loam $\theta = 0.004$

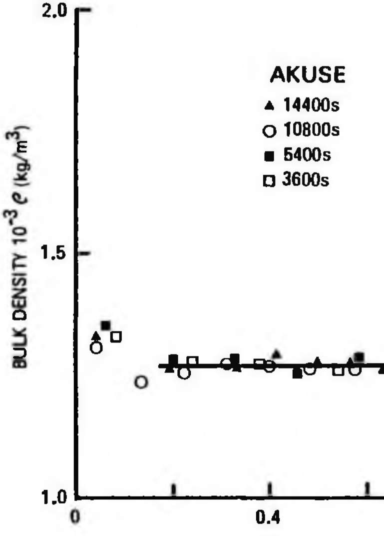
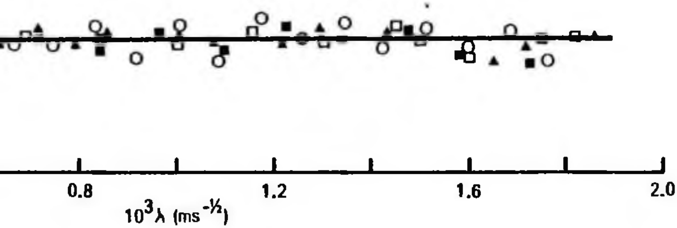

AKUSE
▲ 14400s
○ 10800s
■ 5400s
□ 3600s
BULK DENSITY 10^{-3} ρ (kg/m^3)
2.0
1.5
1.0
0
0.4

Figure 5.8a


0.8
1.2
1.6
2.0
$10^3\lambda$ (ms$^{-½}$)

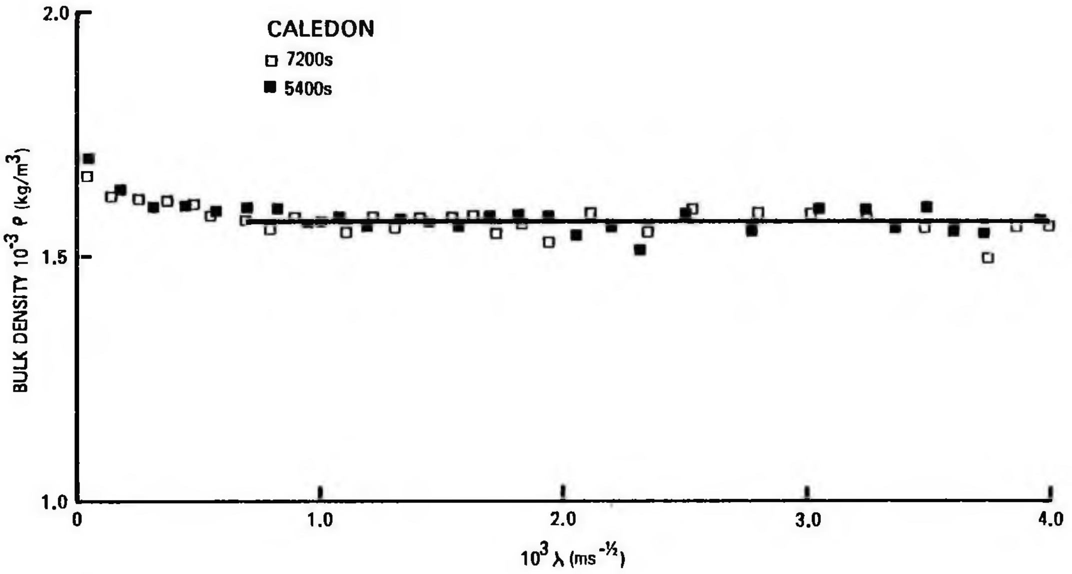

2.0
1.5
1.0
BULK DENSITY 10^{-3} ρ (kg/m^3)
CALEDON
□ 7200s
■ 5400s
0
1.0
2.0
3.0
4.0
10^3 λ (ms$^{-½}$)

Figure 5.8b

of up to 1.7×10^3 kg/m^3.

The plot of θ, c_{Cl^-}, θc_{Cl^-}, and c_{K^+} as a function of λ for Akuse (dry) are presented in figures 5.9a, 5.9b, 5.9c and 5.9d, respectively. It is observed from figure 5.9a that θ at λ=0 of 0.495 is lower than that for the same soil packed moist (figure 5.5a). This difference is the result of air entrapment which is lessened when the soil is initially moist. Also, the difference in λ values between figures 5.5a and 5.9a for Akuse (packed initially moist) and that packed initially dry is firstly the result of the difference in bulk density profiles (mean for Akuse moist is 1.03×10^3 kg/m^3 compared with 1.26×10^3 kg/m^3 for Akuse dry) and secondly due to the fact that the hydraulic conductivity for moist soil is higher than that for dry soil.

Figures 5.9b and 5.9c present some interesting features which we attribute to salt sieving effects. The concentration of Cl^- at λ=0 is significantly lower than the input concentration of 1.0 keq/m^3. At $\lambda = 1.1 \times 10^{-3}$ ms$^{-1/2}$ the concentration distribution starts to increase to a peak greater than 1.0 keq/m^3 just behind the infiltration front. This trend was not expected for in a soil with a low initial water content so that there is very little or no mixing during unsteady unsaturated flow phenomenon induced by sudden availability of KCl solution at the surface of the soil column, one expects no transition zone but a constant concentration equal to the concentration of the solution at the source as was obtained for Caledon sandy loam (figure 5.10b). The low concentration of Cl^- at λ=0 in figure 5.9b could not be due to adsorption of Cl^- because adsorption isotherm conducted showed no Cl^- adsorption for all the concentration range used. It appears then that some of the Cl^-

FIGURE 5.9.

(a) Volumetric water content θ versus λ for Akuse (dry).

(b) Concentration of Cl^- in solution c_{Cl^-} versus λ for Akuse (dry).

(c) Concentration of Cl^- per bulk volume of soil versus λ for Akuse (dry).

(d) Concentration of K^+ in solution as a function of λ for Akuse (dry)

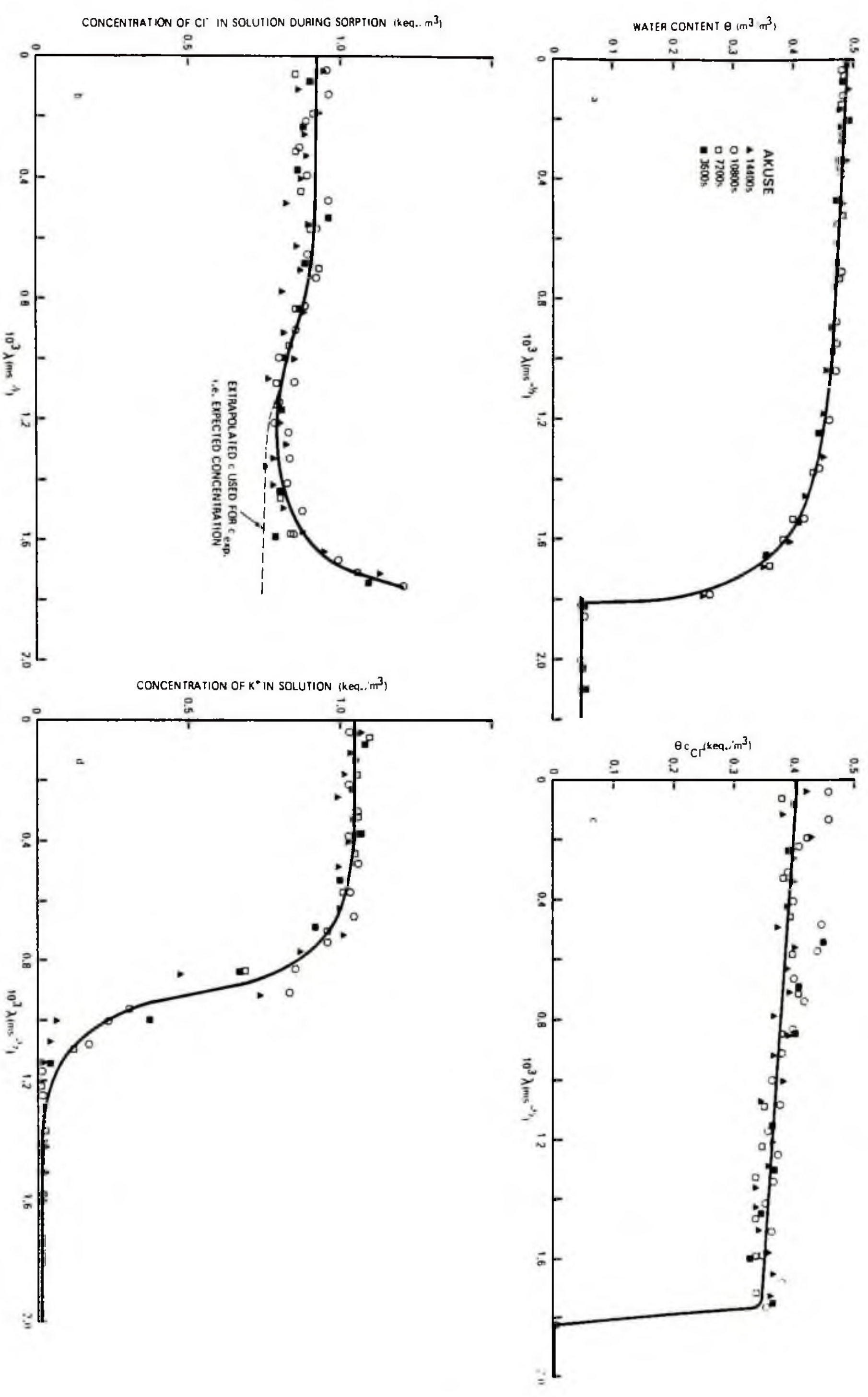

WATER CONTENT θ (m3 m3)
AKUSE
▲ 14400s
○ 10800s
□ 7200s
■ 3600s
θ c Cl (keq./m3)
CONCENTRATION OF Cl⁻ IN SOLUTION DURING SORPTION (keq./m3)
EXTRAPOLATED c USED FOR c exp.
i.e. EXPECTED CONCENTRATION
CONCENTRATION OF K⁺ IN SOLUTION (keq./m3)
10³ λ(ms⁻½)
0
0.1
0.2
0.3
0.4
0.5
1.0
0.8
1.2
1.6
2.0

Figure 5.9

FIGURE 5.10.

(a) Volumetric water content as a function of λ for Caledon sandy loam.

(b) Concentration of Cl^- in solution versus λ for Caledon sandy loam.

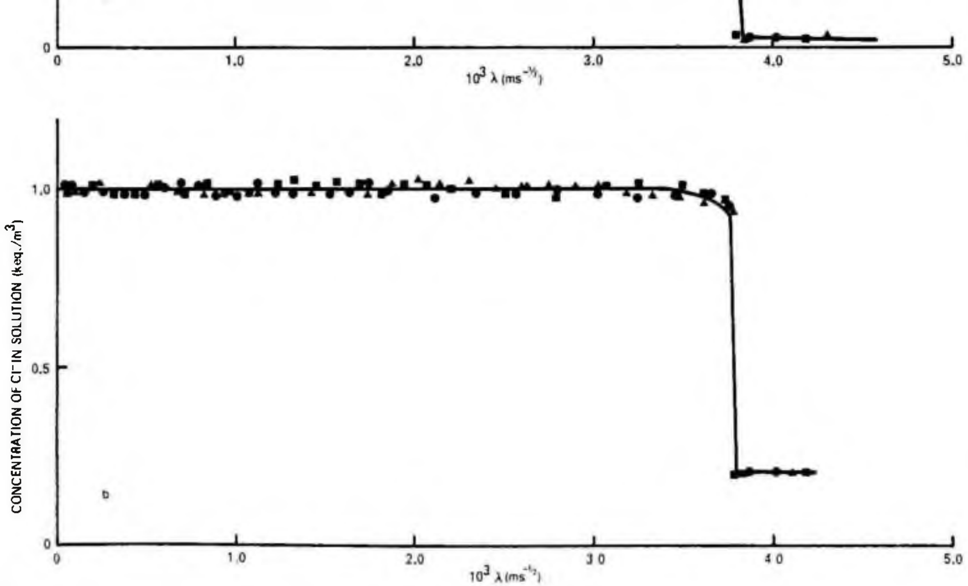
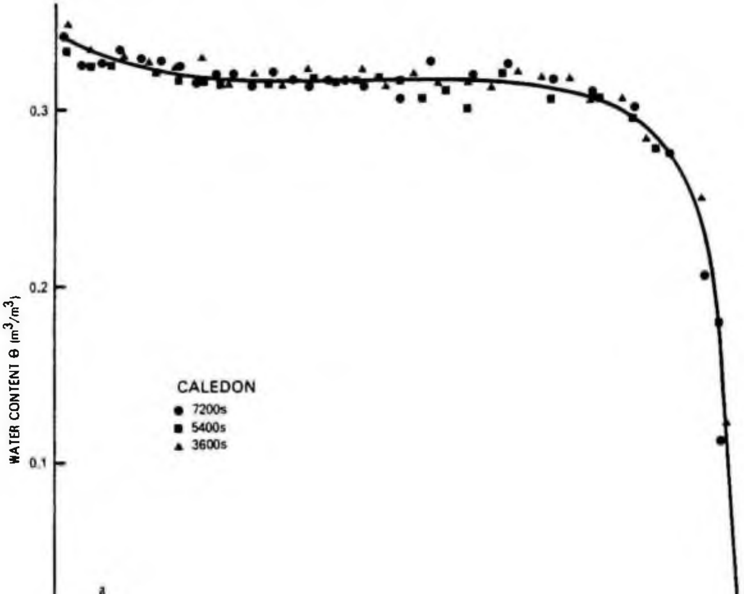

0
1.0
2.0
3.0
4.0
5.0
$10^3\,\lambda\,(ms^{-1/2})$
CONCENTRATION OF Cl⁻ IN SOLUTION (keq./m³)
1.0
0.5
0
b
0
1.0
2.0
3.0
4.0
5.0
$10^3\,\lambda\,(ms^{-1/2})$

Figure 5.10


WATER CONTENT θ (m³/m³)
0.3
0.2
0.1
CALEDON
● 7200s
■ 5400s
▲ 3600s

was excluded at the inlet end. The chloride ions which entered the column of soil, however, were confined to the central more rapidly moving region of each flow path and thereby hastened its passage. At the wetting front where water contents are low, the water together with the Cl^- moved between wedge shaped volumes passing through thin films which sieved the chloride ions thus resulting in accumulation of Cl^- just behind the infiltration front.

Chloride salt balance for the set of experiments reported here was calculated by integrating a plot of θc versus the horizontal distance x for each infiltration run using CSMP. The integrated area multiplied by the surface area of the soil column gave the total quantity of Cl^- in the soil column after infiltration was terminated. This was compared with the total amount of Cl^- in the cumulative quantity of solution that entered the soil column. Table 5.2 which summarizes this comparison indicates that on the average about 7.03% Cl^- was excluded from the soil column.

TABLE 5.2. Chloride Salt Balance for Horizontal Infiltration With Akuse Clay Packed Dry

Infiltration Run #	A keq. Cl^- in soil column after infiltration $\times 10^{-6}$	B keq. Cl^- added through cumulative water infiltrated $\times 10^{-6}$	% Cl^- excluded, i.e. $\frac{(B-A)100}{B}$
1	26.04	27.78	6.26
2	29.26	32.0	8.57
3	45.92	48.82	5.94
4	52.16	56.3	7.35

Comparison between figures 5.9b, 5.9c and 5.9d indicate that at $\lambda=1.4\times10^{-3}$ $ms^{-1/2}$, there is practically no K^+ in solution whereas the Cl^- 'front' is very close to the infiltration front of 1.82×10^{-3} $ms^{-1/2}$. It may be inferred, therefore, that the chloride present between $\lambda\simeq1.0\times10^{-3}$ and $\lambda=1.82\times10^{-3}ms^{-1/2}$ (wetting front) is presumably linked with Ca^{2+}. Conversion of $d\pi/d\lambda$ in equation 3.54 to $dc/d\lambda$ was done using Van't Hoff's law, thus obtaining

$$d\pi/d\lambda = n\ RT\ dc/d\lambda, \text{ where}$$

n for uni-divalent salts is 3. However, because concentration c is measured in equivalents of Cl^- per m^3, $n = 3/2$. Also it must be pointed out that $d\pi/d\lambda$ is the total osmotic pressure gradient. Consequently conversion to $dc/d\lambda$ estimates only the concentration gradient due to Cl^- alone and may over-estimate the osmotic effect. In our experiments the factor β defined earlier was introduced, assuming that in the wet zone where water content is near saturation, compensation between ions occurs so that osmotic pressure gradient in this region may be neglected. Again, the concentration of K^+ at $\lambda=0$ exceeds that of the source by about 5%.

5.4 Derived Data From the Horizontal Infiltration Experiments

The derived data for the dispersion coefficient D_s as a function of θ, calculated for both Cl^- and K^+ using CSMP and equations 3.11b and 3.19 are presented in figures 5.11a and 5.11b. It must be reiterated that the most accurate data in these figures lie between $\theta=0.495$ and

FIGURE 5.11a.

Dispersion coefficient for Cl^- and K^+ plotted as a function of volumetric water content (Akuse clay - moist).

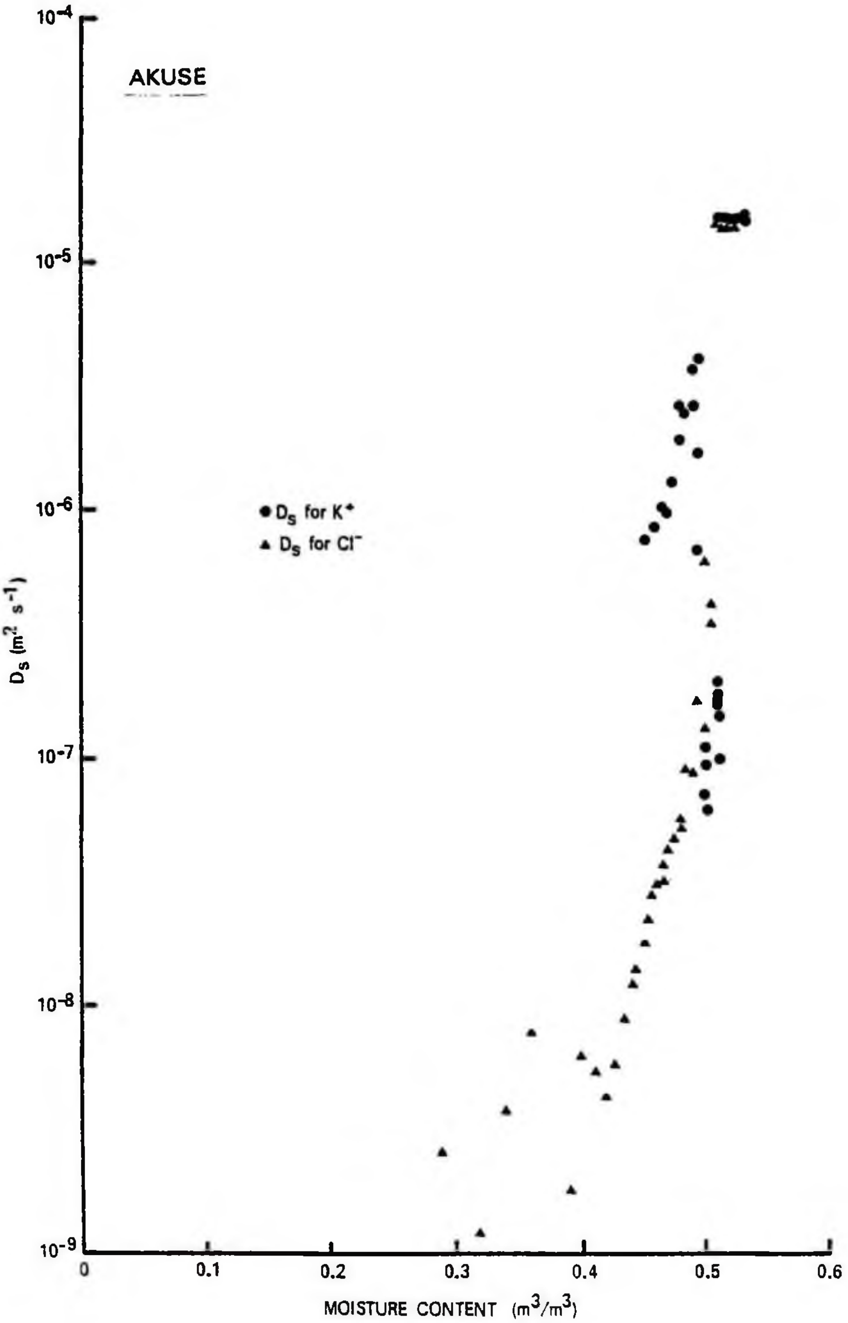

AKUSE
● Ds for K+
▲ Ds for Cl-
Ds (m2 s-1)
10-4
10-5
10-6
10-7
10-8
10-9
0
0.1
0.2
0.3
0.4
0.5
0.6
MOISTURE CONTENT (m3/m3)

Figure 5.11a

FIGURE 5.11b.

Dispersion coefficient for Cl^- and K^+ plotted as a function of volumetric water content (Brookston clay).

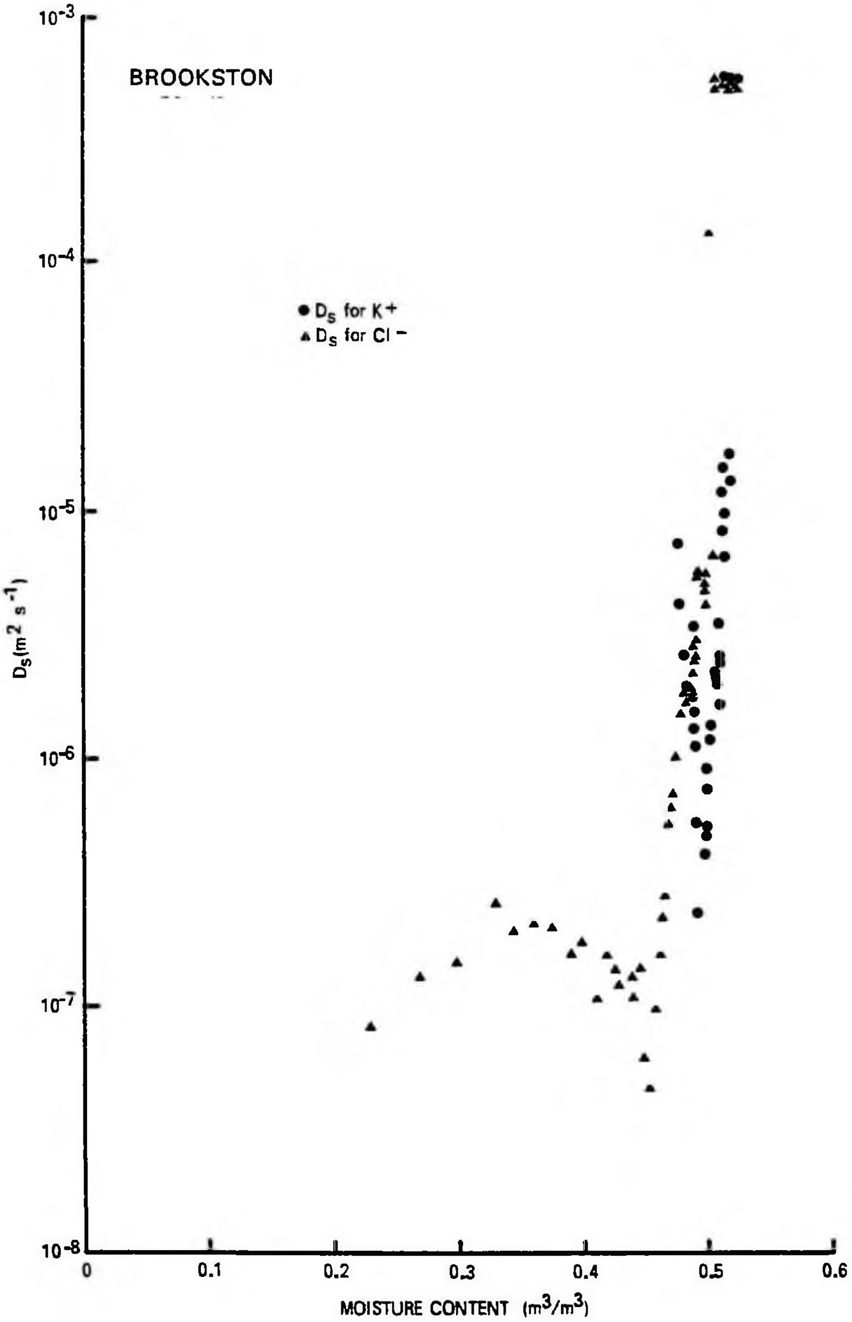

BROOKSTON
● D_s for K^+
▲ D_s for Cl^-
$D_s (m^2 s^{-1})$
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
0
0.1
0.2
0.3
0.4
0.5
0.6
MOISTURE CONTENT (m^3/m^3)

Figure 5.11b

$\theta=0.40$ for Akuse clay and $\theta=0.49$ to $\theta=0.37$ for Brookston clay. Values at the extremes must be less reliable because at these extremes $dc/d\lambda$ tends to zero so that $d\lambda/dc$ becomes infinitely large and also $\int_{\lambda_n}^{\lambda} g \frac{dc}{d\lambda} d\lambda$ tends to zero. Bearing in mind these limitations, however, it is observed from figures 5.11a and 5.11b that the dispersion coefficient data for Cl^- agree fairly well with those for K^+. If adsorption is properly and adequately described, it is to be expected that D_s for Cl^- should be identical with D_s for K^+. This stems from the argument that if we infiltrate a solution of KCl into an inert porous medium, for example sand or glass beads, the D_s calculated for Cl^- in such a system will be the same as that for K^+.

Considering that the molecular diffusivity of KCl in water is about $1.917\text{x}10^{-9}$ m^2s^{-1}, it is concluded that the dispersion coefficient in the soil columns is large and that dispersion in these soil columns is mainly the result of hydrodynamic effects rather than diffusion. It is therefore necessary to re-examine the initial assumption of non-dependence of D_s on the pore water velocity or Darcy flux made in this study. In keeping with Saffman's (1959) analysis, Pfannkuch (1963) found that D_s was independent of Péclet number P_e provided that $P_e \leq 1$ and

$$P_e = u\,l/D_m \qquad (5.6)$$

In equation 5.6, u is the mean pore water velocity, l is a characteristic pore dimension and D_m is the molecular diffusivity of the salt in solution. The Péclet number appropriate to the sorption experiments is formed in a similar way as was done by Smiles and Philip (1978) as follows: u is first identified with the maximum reduced mean pore velocity u^* of equation 5.5 so that equation 5.6 becomes

$$P_e = u^* t^{-1/2}\ l/D_m \tag{5.7}$$

Furthermore, as was done by Saffman (1959), Pfannkuch (1963), and Smiles and Philip (1978), we take l as the 'mean diameter of the grains', and estimate l from the saturated hydraulic conductivity K_o through the use of the Kozeny-Carman relation (Carman, 1939), which yields

$$l = 6\sqrt{5}\ (1-\theta_o)\ [\nu K_o/(g\theta_o{}^3)\ ]^{1/2} \tag{5.8}$$

Equation 5.8 is that of Smiles and Philip (1978) and ν is the kinematic viscosity and g is the acceleration due to gravity. Thus $l=2.38\text{x}10^{-5}$ m for Akuse clay and $l=1.04\text{x}10^{-5}$ m for Brookston clay is inferred from the value of K_o of $2.0\text{x}10^{-5}$ ms^{-1} and $4.0\text{x}10^{-6}$ ms^{-1} for Akuse clay and Brookston clay, respectively (see the hydraulic conductivity versus moisture content curve, figures 5.14a and 5.14b). Taking D_m for KCl as $1.917\text{x}10^{-9}$ m^2s^{-1}, $u^*=1.72\text{x}10^{-3}$ $\text{ms}^{-1/2}$ for Akuse clay and $u^*=6.42\text{x}10^{-4}$ $\text{ms}^{-1/2}$ for Brookston clay (see figures 5.7a and 5.7b), we obtain upon substitution into equation 5.7:

$$P_e = 21.37t^{-1/2} \quad \text{for Akuse clay and}$$
$$P_e = 3.5\ t^{-1/2} \quad \text{for Brookston clay, so that}$$

for Akuse clay

$21.37t^{-1/2} \leq 1$ i.e. $t \geq 7.6$ minutes

and for Brookston clay

$3.5t^{-1/2} \leq 1$ i.e. $t \geq 12.2$ seconds

For these soils, therefore, and under the experimental conditions imposed, D_s is independent of v, except during the initial period of about 10 minutes.

The computed soil moisture diffusivity, D, plotted as a function of $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ for Akuse clay (moist) and Brookston clay are given in figures 5.12a and 5.12b respectively. The high energy moisture characteristic curves for Akuse clay and Brookston clay, used to calculate the hydraulic condutivity K, data (figures 5.14a and 5.14b) are presented in figures 5.13a and 5.13b. The slight differences between water contents at matric potential of zero and $\lambda=0$ (figure 5.5a and 5.6a) is due to air entrapment invariably encountered in horizontal infiltration experiments. These $D(\Theta)$, $D_s(\theta)$ and $K(\Theta)$ data were used to simulate moisture content and salt content profiles for both horizontal infiltration and vertical infiltration.

The dispersion coefficient data for Akuse clay where salt sieving effects are observed (figure 5.15 and Table 5.3) was computed from equation 3.54 and the CSMP listing in Chapter 4. In Table 5.3, THLA is the water content θ, BETA is β defined in Chapter 4, SEEXPT is the expected c, H2 is $D \frac{d\theta}{d\lambda} \frac{dc}{d\lambda}$, Y is the $\int_{\lambda}^{\lambda} (H1-H12+H2-H3)d\lambda$, H7 is $Y\, d\lambda/dc$, H8 is the osmosis term $\frac{3RTc\sigma K(\theta)\beta}{2g\rho_w}$ and DS is the dispersion coefficient. As indicated earlier the introduction of β assumes that in the wet region osmosis is very small and that osmotic effects

FIGURE 5.12.

(a) Soil moisture diffusivity as a function of $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$, Akuse clay (moist).

(b) Soil moisture diffusivity as a function of $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$. Brookston clay.

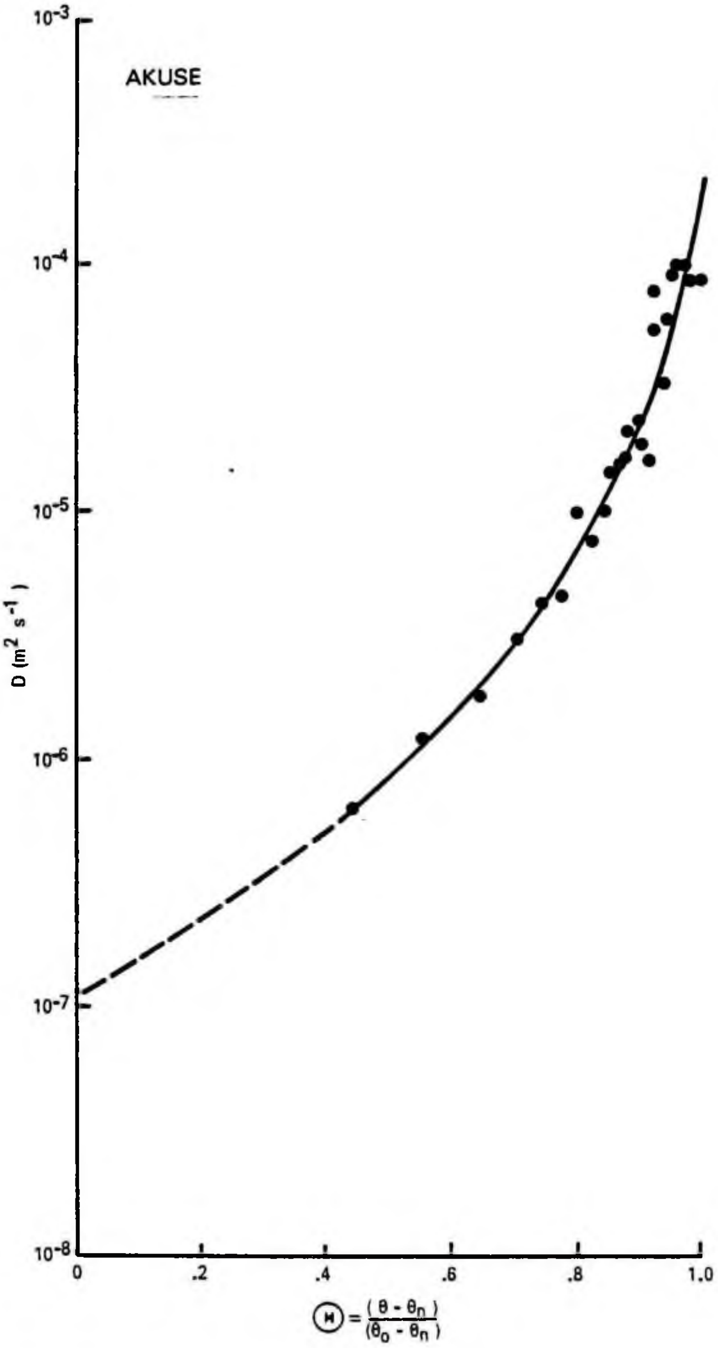

AKUSE
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
D ($m^2 s^{-1}$)
0
.2
.4
.6
.8
1.0
$\Theta = \frac{(\theta - \theta_n)}{(\theta_o - \theta_n)}$

Figure 5.12a

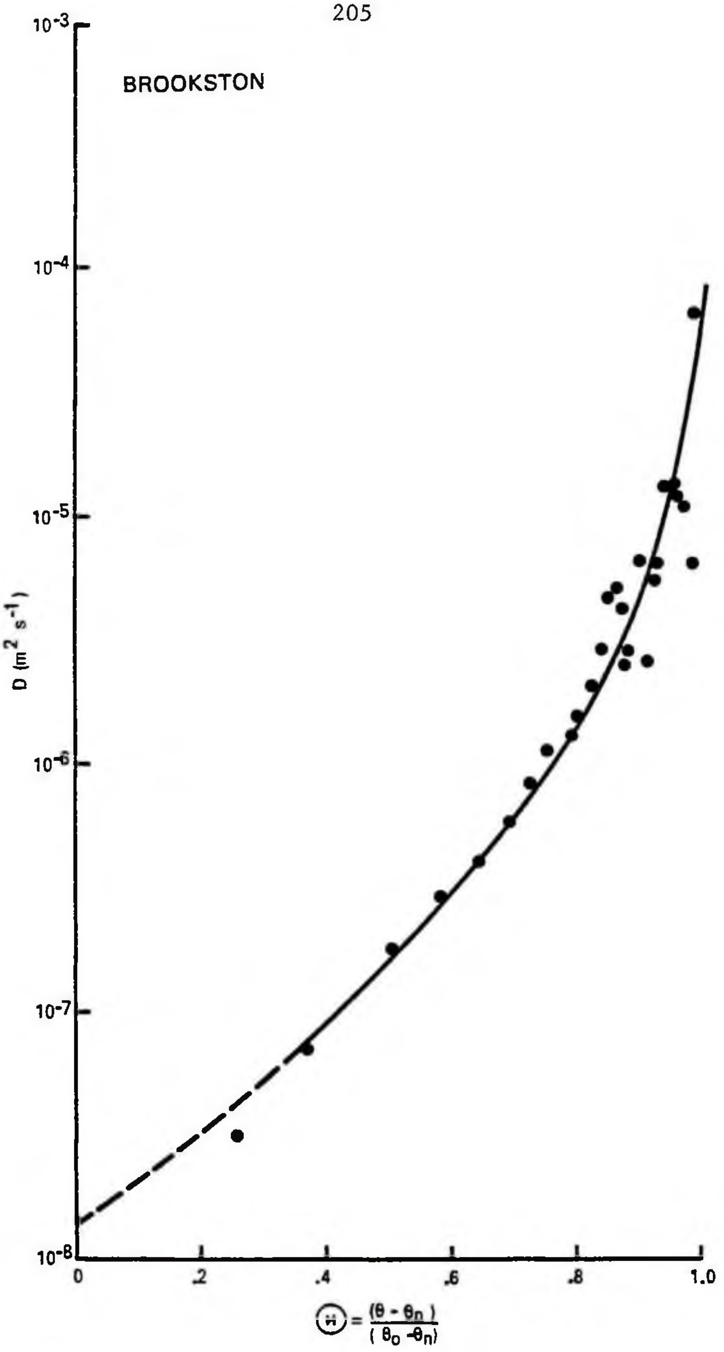

BROOKSTON
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
D ($m^2 s^{-1}$)
0
.2
.4
.6
.8
1.0
$\Theta = \frac{(\theta - \theta_n)}{(\theta_o - \theta_n)}$

Figure 5.12b

FIGURE 5.13.

(a) High energy moisture characteristic curves for wetting (w) and draining (d) cycles, Akuse clay.

(b) High energy moisture characteristic curves for wetting (w) and desorption (d) cyles, Brookston clay.

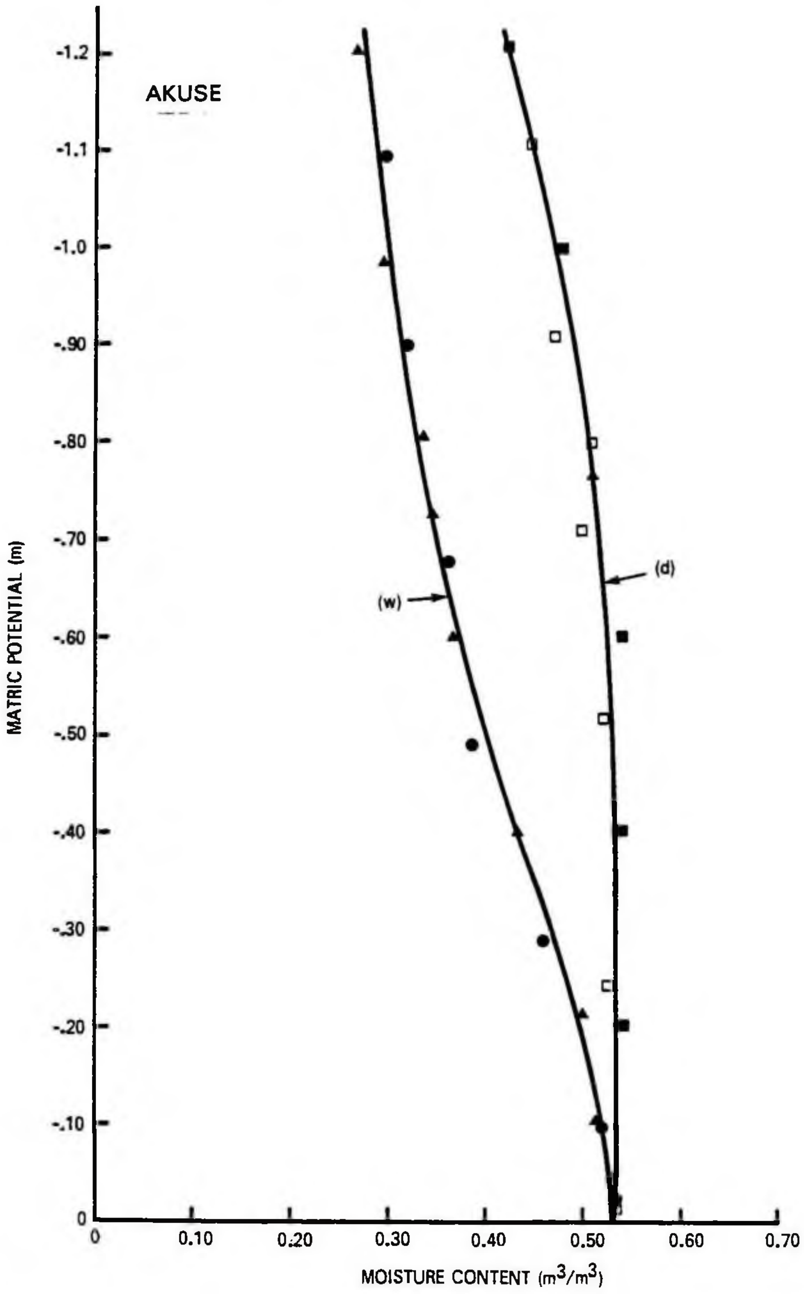

AKUSE
MATRIC POTENTIAL (m)
-1.2
-1.1
-1.0
-.90
-.80
-.70
-.60
-.50
-.40
-.30
-.20
-.10
0
0
0.10
0.20
0.30
0.40
0.50
0.60
0.70
MOISTURE CONTENT (m3/m3)
(w)
(d)

Figure 5.13a

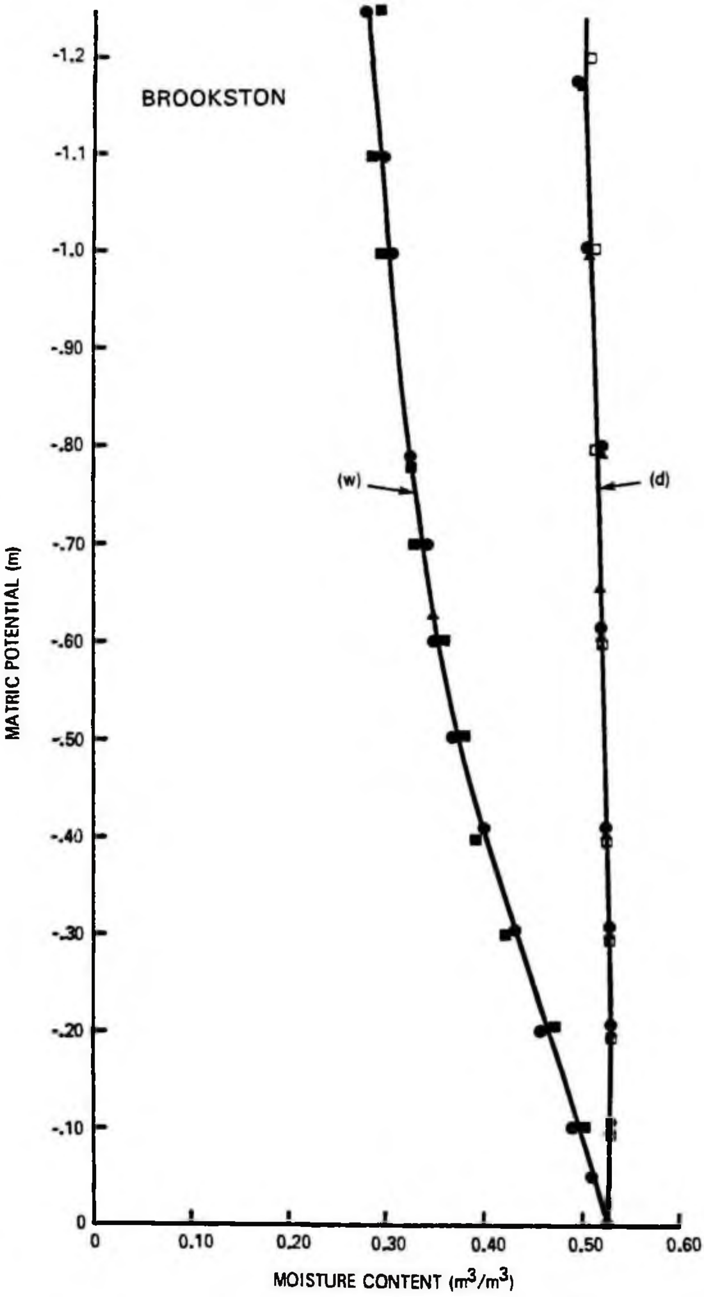

BROOKSTON
MATRIC POTENTIAL (m)
-1.2
-1.1
-1.0
-.90
-.80
-.70
-.60
-.50
-.40
-.30
-.20
-.10
0
(w)
(d)
0
0.10
0.20
0.30
0.40
0.50
0.60
MOISTURE CONTENT (m^3/m^3)

Figure 5.13b

FIGURE 5.14.

(a) Hydraulic conductivity K as a function of $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ for Akuse clay.

(b) Hydraulic conductivity K as a function of $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ for Brookston clay.

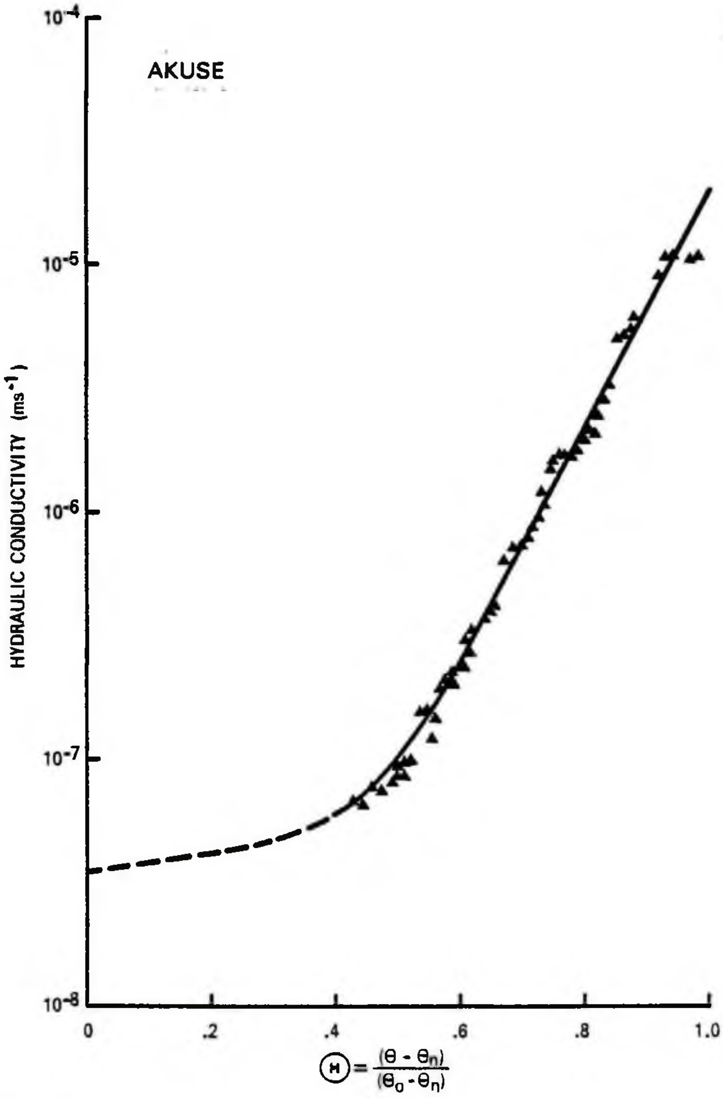

AKUSE
HYDRAULIC CONDUCTIVITY (ms^{-1})
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
0
.2
.4
.6
.8
1.0
$\Theta = \frac{(\theta - \theta_n)}{(\theta_o - \theta_n)}$

Figure 5.14a

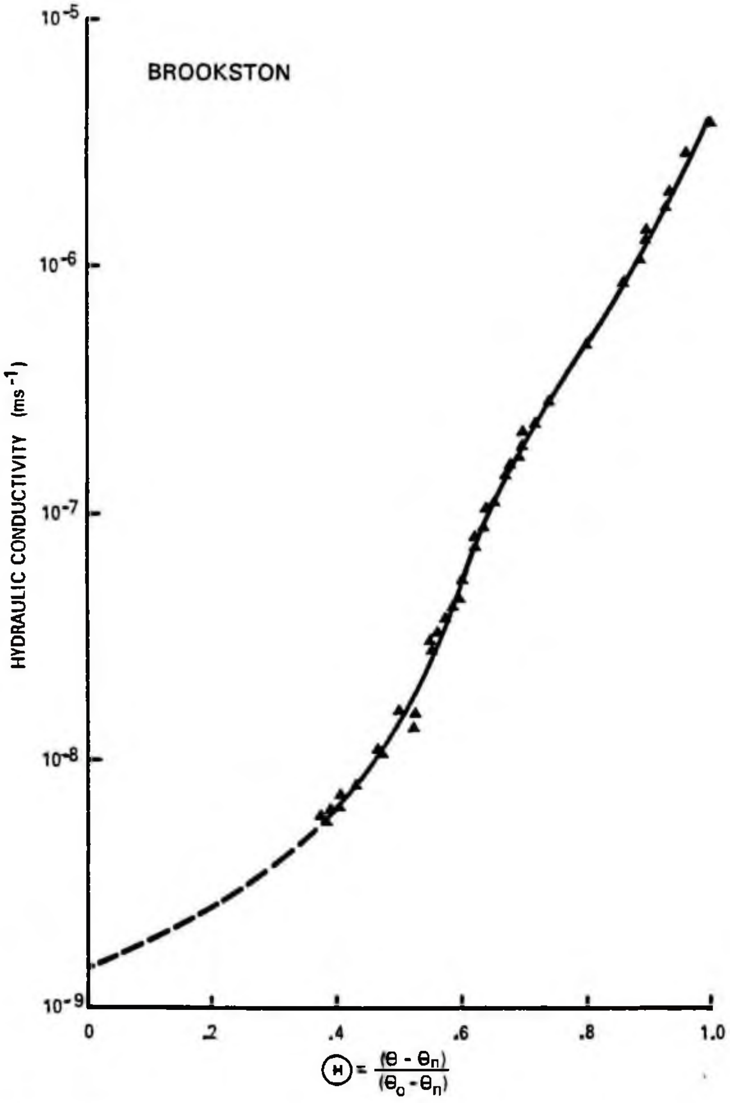

BROOKSTON
HYDRAULIC CONDUCTIVITY (ms^{-1})
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
0
.2
.4
.6
.8
1.0
$\Theta = \frac{(\theta - \theta_n)}{(\theta_o - \theta_n)}$

Figure 5.14b

FIGURE 5.15.

Dispersion coefficient for Cl^- and with salt sieving effects accounted for, plotted as a function of volumetric water content (Akuse, dry).

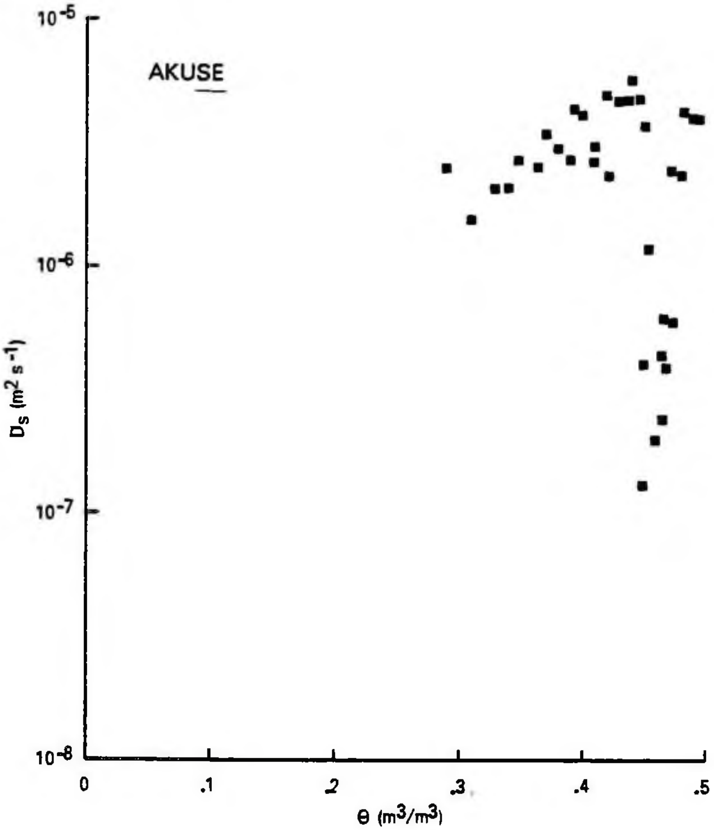


Figure 5.15

dominate at the wetting front. We have to reiterate that negative D_s values are obtained at λ values greater than 1.2×10^{-3} $ms^{-1/2}$ if salt sieving and osmosis effects are not considered in the calculation of D_s (see Table 5.4). This is because from $\lambda = 1.2 \times 10^{-3}$ $ms^{-1/2}$ onwards (figure 5.9b), $dc/d\lambda > 0$. Introduction of the salt sieving and osmosis terms result in positive D_s values for all λ values. However, for greater reliability of data presented in figure 5.15, it is necessary to devise a method to determine the total salt concentration gradient during the infiltration run. Note that the D_s values in Table 5.4 are slightly larger than those in Table 5.3. This is so because

H12 $\left(= \frac{\lambda\,\theta_{ex}}{2}\,\frac{dc}{d\lambda}\right)$ is zero when salt sieving effect is not included in the calculation of D_s. Data in figure 5.15 for D_s (with salt sieving effect accounted for) plotted as a function of θ shows a minimum at $\theta = 0.45$. Smiles *et al*. (1978) observed a similar minimum in D_s plotted against θ for their experimental soil. This minimum in D_s may be attributed to an artifact introduced by the correction term β, especially when we consider that the extrapolated curve (figure 5.9b) for expected c is arbitrary.

5.5 Simulated $\theta(\lambda)$ and $c(\lambda)$ Results for Horizontal Infiltration Experiments

The simulated $\theta(\lambda)$ relationship calculated from $D(\lambda)$ results which were in turn derived from smoothed experimental $\theta(\lambda)$ data is presented in figures 5.16a and 5.16b for Akuse clay and Brookston clay, respectively. Tables 5.5a and 5.5b are the computer output of the data

TABLE 5.3. Computer output showing positive D_s values due to inclusion of salt sieving term in equation 3.54. Explanation of the other output headings is in the text.

```
CSMP                                                          SIMP      INTEGRATION

  LANDA        THLA         BETA           SEEXPT       H2           Y            H7           H8             DS
0.0          4.9500E-01   0.0            9.3000E-01   3.5877E-06  -2.0160E-06   2.0160E-02   0.0            4.0728E-02
3.6400E-03   4.9136E-01   0.0            9.2964E-01   3.6948E-06  -2.0493E-06   1.9897E-02   0.0            4.0494E-02
7.2800E-03   4.8886E-01   0.0            9.2927E-01   3.4890E-06  -2.0752E-06   2.1333E-02   0.0            4.3639E-02
1.0920E-02   4.8727E-01   0.0            9.2891E-01   3.2831E-06  -2.0950E-06   2.2883E-02   0.0            4.6962E-02
1.4560E-02   4.8636E-01   0.0            9.2854E-01   3.4877E-06  -2.1105E-06   2.1656E-02   0.0            4.4609E-02
1.8200E-02   4.8545E-01   0.0            9.2818E-01   3.6921E-06  -2.1257E-06   2.0639E-02   0.0            4.2514E-02
2.1840E-02   4.8463E-01   0.0            9.2763E-01   6.9382E-06  -2.1450E-06   1.1080E-02   0.0            2.2862E-02
2.5480E-02   4.8390E-01   0.0            9.2690E-01   6.9024E-06  -2.1682E-06   1.1255E-02   0.0            2.3259E-02
2.9120E-02   4.8318E-01   0.0            9.2618E-01   6.6613E-06  -2.1908E-06   1.1781E-02   0.0            2.4382E-02
3.2760E-02   4.8217E-01   0.0            9.2545E-01   7.1706E-06  -2.2142E-06   1.1036E-02   0.0            2.2930E-02
3.6400E-02   4.8108E-01   0.0            9.2472E-01   7.1327E-06  -2.2372E-06   1.1224E-02   0.0            2.3332E-02
4.0040E-02   4.7999E-01   0.0            9.2399E-01   7.0604E-06  -2.2595E-06   1.1446E-02   0.0            2.3846E-02
4.3680E-02   4.7908E-01   0.0            9.2326E-01   6.9203E-06  -2.2802E-06   1.1778E-02   0.0            2.4585E-02
4.7320E-02   4.7817E-01   0.0            9.2254E-01   6.9163E-06  -2.3004E-06   1.1882E-02   0.0            2.4849E-02
5.0960E-02   4.7726E-01   0.0            9.2181E-01   7.2865E-06  -2.3198E-06   1.1367E-02   0.0            2.3816E-02
5.4600E-02   4.7635E-01   0.0            9.2108E-01   7.2476E-06  -2.3385E-06   1.1512E-02   0.0            2.4167E-02
5.8240E-02   4.7544E-01   0.0            9.2035E-01   7.0723E-06  -2.3563E-06   1.1879E-02   0.0            2.4985E-02
6.1880E-02   4.7453E-01   0.0            9.1812E-01   3.5742E-05  -2.4021E-06   2.3943E-03   0.0            5.0456E-03
6.5520E-02   4.7362E-01   0.0            9.1448E-01   3.5374E-05  -2.4727E-06   2.4683E-03   0.0            5.2538E-03
6.9160E-02   4.7271E-01   0.0            9.1084E-01   3.5445E-05  -2.5402E-06   2.5489E-03   0.0            5.3920E-03
7.2800E-02   4.7180E-01   0.0            9.0580E-01   5.3069E-05  -2.6281E-06   1.7596E-03   0.0            3.7299E-03
7.6440E-02   4.7089E-01   0.0            9.0034E-01   5.3289E-05  -2.7191E-06   1.8114E-03   0.0            3.8468E-03
8.0080E-02   4.6998E-01   0.0            8.9492E-01   3.4397E-05  -2.8053E-06   2.9924E-03   0.0            6.1642E-03
8.3720E-02   4.6907E-01   0.0            8.9128E-01   3.5408E-05  -2.8607E-06   2.8622E-03   0.0            6.1019E-03
8.7360E-02   4.6816E-01   0.0            8.8292E-01   1.0007E-04  -2.9781E-06   9.9357E-04   0.0            2.1223E-03
9.1000E-02   4.6725E-01   0.0            8.7300E-01   7.0623E-05  -3.1105E-06   1.5569E-03   0.0            3.3320E-03
9.4640E-02   4.6634E-01   0.0            8.6572E-01   7.0539E-05  -3.2022E-06   1.6027E-03   0.0            3.4369E-03
9.8280E-02   4.6543E-01   0.0            8.5516E-01   1.0579E-04  -3.3262E-06   1.1086E-03   0.0            2.3819E-03
1.0192E-01   4.6404E-01   0.0            8.4616E-01   7.0480E-05  -3.4261E-06   1.7107E-03   0.0            3.6866E-03
1.0556E-01   4.6222E-01   0.0            8.3776E-01   1.4051E-04  -3.5138E-06   8.7767E-04   0.0            1.8988E-03
1.0920E-01   4.6040E-01   0.0            8.2320E-01   1.3982E-04  -3.6518E-06   9.1411E-04   0.0            1.9855E-03
1.1284E-01   4.5858E-01   3.4754E-03     8.1432E-01   3.4880E-05  -3.7061E-06   3.7081E-03   2.1657E-03     1.2809E-02
1.1648E-01   4.5676E-01   7.9654E-03     8.0704E-01   3.4709E-05  -3.7368E-06   3.7460E-03   4.9630E-03     1.9067E-02
1.2012E-01   4.5488E-01   1.2640E-02     7.9988E-01  -6.7543E-05  -3.7629E-06  -1.9322E-03   3.1730E-03     2.7277E-03
1.2376E-01   4.5124E-01   2.1530E-02     7.9624E-01  -3.4541E-05  -3.7441E-06  -3.7355E-03   6.7237E-03     6.6222E-03
1.2740E-01   4.4760E-01   3.0340E-02     7.9260E-01  -3.4345E-05  -3.7278E-06  -3.7157E-03   9.1312E-03     1.2099E-02
1.3104E-01   4.4413E-01   3.9072E-02     7.8896E-01  -3.4008E-05  -3.7126E-06  -3.7050E-03   1.4642E-02     2.4625E-02
1.3468E-01   4.4110E-01   4.7728E-02     7.8532E-01  -3.3806E-05  -3.7013E-06  -3.6928E-03   1.8478E-02     3.3518E-02
1.3832E-01   4.3710E-01   5.6307E-02     7.8168E-01  -3.3517E-05  -3.6920E-06  -3.6940E-03   1.5114E-02     2.6127E-02
1.4196E-01   4.3206E-01   6.5911E-02     7.7804E-01  -4.9746E-05  -3.6829E-06  -2.4566E-03   1.7843E-02     3.5011E-02
1.4560E-01   4.2660E-01   7.6336E-02     7.7440E-01  -4.9159E-05  -3.6748E-06  -2.4512E-03   1.9353E-02     3.9619E-02
1.4924E-01   4.2114E-01   8.6626E-02     7.7076E-01  -4.8587E-05  -3.6698E-06  -2.4463E-03   2.0637E-02     4.3194E-02
1.5288E-01   4.1136E-01   1.0438E-01     7.6712E-01  -1.2668E-04  -3.6649E-06  -9.1564E-04   1.1099E-02     2.4755E-02
1.5652E-01   4.0044E-01   1.2809E-01     7.6348E-01  -2.1566E-04  -3.6683E-06  -5.2397E-04   1.6416E-02     3.9686E-02
1.6016E-01   3.8928E-01   1.5714E-01     7.5992E-01  -3.2591E-04  -3.6865E-06  -3.3846E-04   1.0401E-02     2.5849E-02
1.6380E-01   3.7290E-01   1.9179E-01     7.5810E-01  -2.8594E-04  -3.7307E-06  -3.7310E-04   1.3274E-02     3.4595E-02
1.6744E-01   3.5286E-01   2.2772E-01     7.5628E-01  -3.2346E-04  -3.7988E-06  -3.1633E-04   9.9347E-03     2.7258E-02
1.7108E-01   3.2724E-01   2.7356E-01     7.5410E-01  -6.4428E-04  -3.9206E-06  -1.5070E-04   6.8659E-03     2.0521E-02
1.7472E-01   2.9266E-01   3.3694E-01     7.5107E-01  -5.6023E-04  -4.1437E-06  -1.5936E-04   7.5452E-03     2.5237E-02
1.7836E-01   2.2280E-01   3.7298E-01     4.5893E-01   3.0956E-03  -2.5890E-06   1.3054E-05   2.7010E 01     1.2123E 02
1.8200E-01   5.0000E-02   0.0            1.0000E-02   0.0          0.0          0.0          0.0            0.0


KDN2,KGN4=   0.808535E-01   -0.201602E-05
```

TABLE 5.4 . Computer output showing both positive and negative D_s values because salt sieving term was omitted by setting $\sigma=0$.

```
CSMP                                                                     SIMF     INTEGRATION

 LAMDA        THLA         BETA          SEEXPT       H2           Y            H7           H8              DS
 0.0          4.9500E-01   0.0           9.3000E-01   3.5877E-06  -2.5595E-06   2.5595E-02   0.0             5.1708E-02
 3.6400E-03   4.9136E-01   0.0           9.2964E-01   3.6948E-06  -2.5721E-06   2.4973E-02   0.0             5.0824E-02
 7.2800E-03   4.8886E-01   0.0           9.2927E-01   3.4890E-06  -2.5842E-06   2.6566E-02   0.0             5.4342E-02
 1.0920E-02   4.8727E-01   0.0           9.2891E-01   3.2831E-06  -2.5957E-06   2.8352E-02   0.0             5.8186E-02
 1.4560E-02   4.8636E-01   0.0           9.2854E-01   3.4877E-06  -2.6070E-06   2.6800E-02   0.0             5.5103E-02
 1.8200E-02   4.8545E-01   0.0           9.2818E-01   3.6921E-06  -2.6180E-06   2.5419E-02   0.0             5.2361E-02
 2.1840E-02   4.8463E-01   0.0           9.2763E-01   6.9392E-06  -2.6343E-06   1.3607E-02   0.0             2.8077E-02
 2.5480E-02   4.8390E-01   0.0           9.2690E-01   6.9024E-06  -2.6556E-06   1.3785E-02   0.0             2.8487E-02
 2.9120E-02   4.8318E-01   0.0           9.2618E-01   6.6013E-06  -2.6762E-06   1.4391E-02   0.0             2.9784E-02
 3.2760E-02   4.8217E-01   0.0           9.2545E-01   7.1706E-06  -2.6904E-06   1.3464E-02   0.0             2.7923E-02
 3.6400E-02   4.8108E-01   0.0           9.2472E-01   7.1327E-06  -2.7158E-06   1.3626E-02   0.0             2.8323E-02
 4.0040E-02   4.7999E-01   0.0           9.2399E-01   7.0604E-06  -2.7346E-06   1.3853E-02   0.0             2.8860E-02
 4.3680E-02   4.7908E-01   0.0           9.2326E-01   6.9203E-06  -2.7528E-06   1.4219E-02   0.0             2.9681E-02
 4.7320E-02   4.7817E-01   0.0           9.2254E-01   6.9163E-06  -2.7705E-06   1.4311E-02   0.0             2.9928E-02
 5.0960E-02   4.7726E-01   0.0           9.2181E-01   7.2865E-06  -2.7875E-06   1.3658E-02   0.0             2.8618E-02
 5.4600E-02   4.7635E-01   0.0           9.2108E-01   7.2476E-06  -2.8039E-06   1.3803E-02   0.0             2.8977E-02
 5.8240E-02   4.7544E-01   0.0           9.2035E-01   7.0723E-06  -2.8195E-06   1.4214E-02   0.0             2.9896E-02
 6.1880E-02   4.7453E-01   0.0           9.1812E-01   3.5742E-05  -2.8661E-06   2.8568E-03   0.0             6.0202E-03
 6.5520E-02   4.7362E-01   0.0           9.1448E-01   3.5374E-05  -2.9402E-06   2.9587E-03   0.0             6.2471E-03
 6.9160E-02   4.7271E-01   0.0           9.1084E-01   3.5445E-05  -3.0110E-06   3.0214E-03   0.0             6.3916E-03
 7.2800E-02   4.7180E-01   0.0           9.0580E-01   5.3069E-05  -3.1047E-06   2.0789E-03   0.0             4.4062E-03
 7.6440E-02   4.7089E-01   0.0           9.0034E-01   5.0289E-05  -3.2019E-06   2.1330E-03   0.0             4.5298E-03
 8.0080E-02   4.6998E-01   0.0           8.9492E-01   3.4397E-05  -3.2939E-06   3.3962E-03   0.0             7.2262E-03
 8.3720E-02   4.6907E-01   0.0           8.9128E-01   3.5408E-05  -3.3521E-06   3.3540E-03   0.0             7.1502E-03
 8.7360E-02   4.6816E-01   0.0           8.8292E-01   1.0607E-04  -3.4791E-06   1.1607E-03   0.0             2.4793E-03
 9.1000E-02   4.6725E-01   0.0           8.7300E-01   7.0623E-05  -3.6228E-06   1.8133E-03   0.0             3.8807E-03
 9.4640E-02   4.6634E-01   0.0           8.6572E-01   7.0539E-05  -3.7217E-06   1.8627E-03   0.0             3.9944E-03
 9.8280E-02   4.6543E-01   0.0           8.5516E-01   1.0579E-04  -3.8564E-06   1.2854E-03   0.0             2.7617E-03
 1.0192E-01   4.6404E-01   0.0           8.4616E-01   7.0480E-05  -3.9638E-06   1.9792E-03   0.0             4.2651E-03
 1.0556E-01   4.6222E-01   0.0           8.3776E-01   1.4051E-04  -4.0567E-06   1.0133E-03   0.0             2.1922E-03
 1.0920E-01   4.6040E-01   0.0           8.2320E-01   1.3932E-04  -4.2060E-06   1.0528E-03   0.0             2.2867E-03
 1.1284E-01   4.5858E-01   3.4754E-03    8.1432E-01   3.4880E-05  -4.2627E-06   4.2651E-03   0.0             9.3006E-03
 1.1648E-01   4.5676E-01   7.9654E-03    8.0704E-01   3.4709E-05  -4.2937E-06   4.3043E-03   0.0             9.4234E-03
 1.2012E-01   4.5488E-01   1.2640E-02    7.9988E-01  -6.7543E-05  -4.3197E-06  -2.2182E-03   0.0            -4.8764E-03
 1.2376E-01   4.5124E-01   2.1530E-02    7.9624E-01  -3.4541E-05  -4.2939E-06  -4.2840E-03   0.0            -9.4939E-03
 1.2740E-01   4.4760E-01   3.0340E-02    7.9260E-01  -3.4345E-05  -4.2714E-06  -4.2575E-03   0.0            -9.5118E-03
 1.3104E-01   4.4413E-01   3.9072E-02    7.8896E-01  -3.4088E-05  -4.2518E-06  -4.2420E-03   0.0            -9.5511E-03
 1.3468E-01   4.4110E-01   4.7728E-02    7.8532E-01  -3.3886E-05  -4.2352E-06  -4.2254E-03   0.0            -9.5792E-03
 1.3832E-01   4.3710E-01   5.6307E-02    7.8168E-01  -3.3517E-05  -4.2215E-06  -4.2239E-03   0.0            -9.6634E-03
 1.4196E-01   4.3206E-01   6.5911E-02    7.7804E-01  -4.9746E-05  -4.2081E-06  -2.8070E-03   0.0            -6.4967E-03
 1.4560E-01   4.2660E-01   7.6336E-02    7.7440E-01  -4.9159E-05  -4.1964E-06  -2.7992E-03   0.0            -6.5615E-03
 1.4924E-01   4.2114E-01   8.6626E-02    7.7076E-01  -4.8537E-05  -4.1890E-06  -2.7924E-03   0.0            -6.6306E-03
 1.5288E-01   4.1136E-01   1.0438E-01    7.6712E-01  -1.2668E-04  -4.1822E-06  -1.0449E-03   0.0            -2.5400E-03
 1.5652E-01   4.0044E-01   1.2809E-01    7.6348E-01  -2.1566E-04  -4.1863E-06  -5.9797E-04   0.0            -1.4933E-03
 1.6016E-01   3.8928E-01   1.5714E-01    7.5992E-01  -3.2591E-04  -4.2096E-06  -3.8649E-04   0.0            -9.9284E-04
 1.6380E-01   3.7290E-01   1.9179E-01    7.5810E-01  -2.3594E-04  -4.2680E-06  -4.2683E-04   0.0            -1.1446E-03
 1.6744E-01   3.5286E-01   2.2772E-01    7.5628E-01  -3.2346E-04  -4.3625E-06  -3.6328E-04   0.0            -1.0295E-03
 1.7108E-01   3.2724E-01   2.7356E-01    7.5410E-01  -6.4128E-04  -4.5365E-06  -1.7438E-04   0.0            -5.3288E-04
 1.7472E-01   2.9266E-01   3.3694E-01    7.5107E-01  -5.5623E-04  -4.8692E-06  -1.8726E-04   0.0            -6.3986E-04
 1.7836E-01   2.2280E-01   3.7298E-01    4.5893E-01   3.0936E-03  -3.2600E-06   1.6134E-05   0.0             7.2417E-05
 1.8200E-01   5.0000E-02   0.0           1.0000E-02   0.0          0.0          0.0          0.0             0.0


KON2,KON4=   0.808535E-01   -2.255954E-05
```

plotted in figures 5.16a and 5.16b, included to show the degree of agreement between experimental and simulated $\theta(\lambda)$ data. In Tables 5.5a and 5.5b, THLA is the experimental water content and THETA2 is the simulated water content. $d\theta/d\lambda$ which was calculated with the DERIV algorithm of CSMP was integrated to obtain THETA1 which is compared with both THLA and THETA2 to ascertain the accuracy of the calculation of $d\theta/d\lambda$. Interpolation of the smoothed experimental $\theta(\lambda)$ data was done by Lagrange quadratic interpolation algorithm of CSMP. These interpolated $\theta(\lambda)$ data (THLA in Tables 5.5a and 5.5b) are also plotted in figures 5.16a and 5.16b. It is observed that excellent agreement is obtained between simulated $\theta(\lambda)$ and experimental $\theta(\lambda)$ data. Given $D(\theta)$ or $D(\lambda)$ therefore, $\theta(\lambda)$ can be predicted or simulated with a very good degree of accuracy using the computer program described in Chapter 4.

Simulated $c(\lambda)$ relationship computed from $D_s(\lambda)$ data which were calculated from smoothed experimental $c(\lambda)$ data for chloride is given in figures 5.17a and 5.17b for Akuse clay and Brookston clay, respectively. $c(\lambda)$ relationship computed using CSMP program for the analytical solution (equation 3.21) is also plotted in figures 5.17a and 5.17b which also show simulated $c(\lambda)$ data obtained with constant values of θD_s chosen from upper, middle and lower D_s range of figures 5.11a and 5.11b. Tables 5.6a and 5.6b also present computer output of the data plotted in figures 5.17a and 5.17b. Tables 5.6a and 5.6b have been included to show clearly the minor differences (which do not appear in the graphical representations, figures 5.17a and 5.17b) between $c(\lambda)$ data calculated analytically, $c(\lambda)$ interpolated from experimental data and $c(\lambda)$ computed non-analytically using the algorithm described in Appendix D. In

FIGURE 5.16.

(a) Simulated water content as a function of λ (Akuse clay). Interpolated experimental data points are provided for comparison.

(b) Simulated water content as a function of λ (Brookston clay).

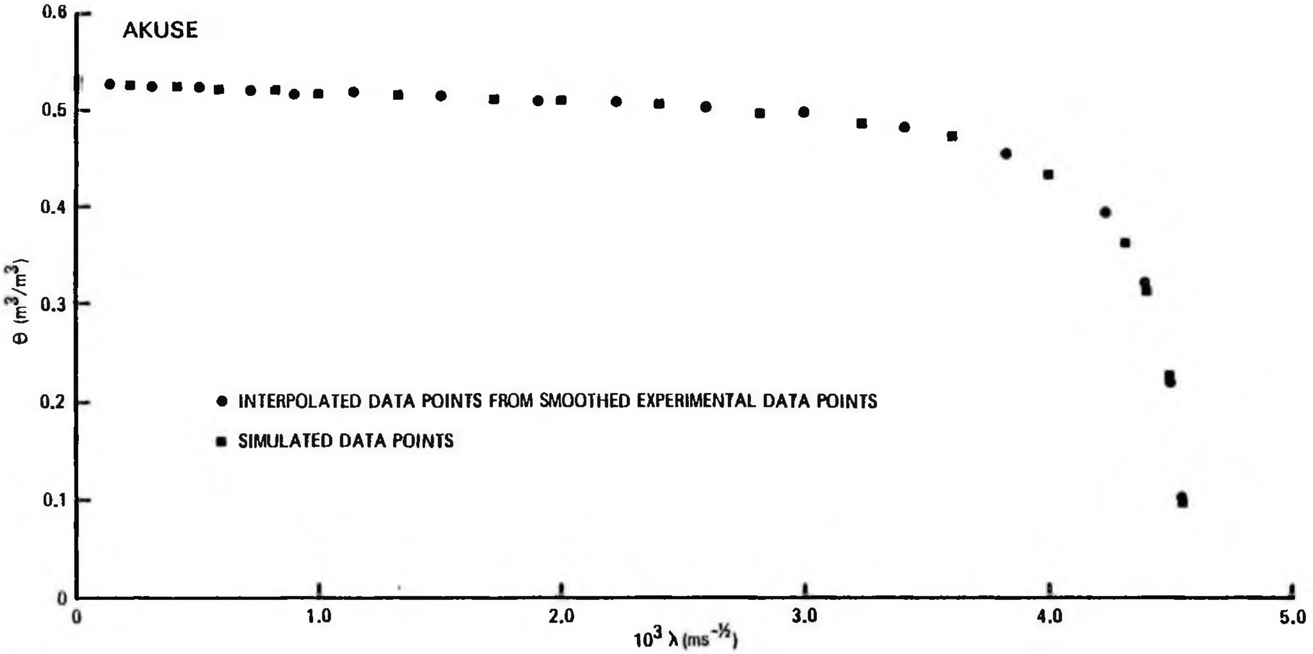

AKUSE
● INTERPOLATED DATA POINTS FROM SMOOTHED EXPERIMENTAL DATA POINTS
■ SIMULATED DATA POINTS
0.6
0.5
0.4
0.3
0.2
0.1
0
$\theta\ (m^3/m^3)$
0
1.0
2.0
3.0
4.0
5.0
$10^3\ \lambda\ (ms^{-1/2})$

Figure 5.16a

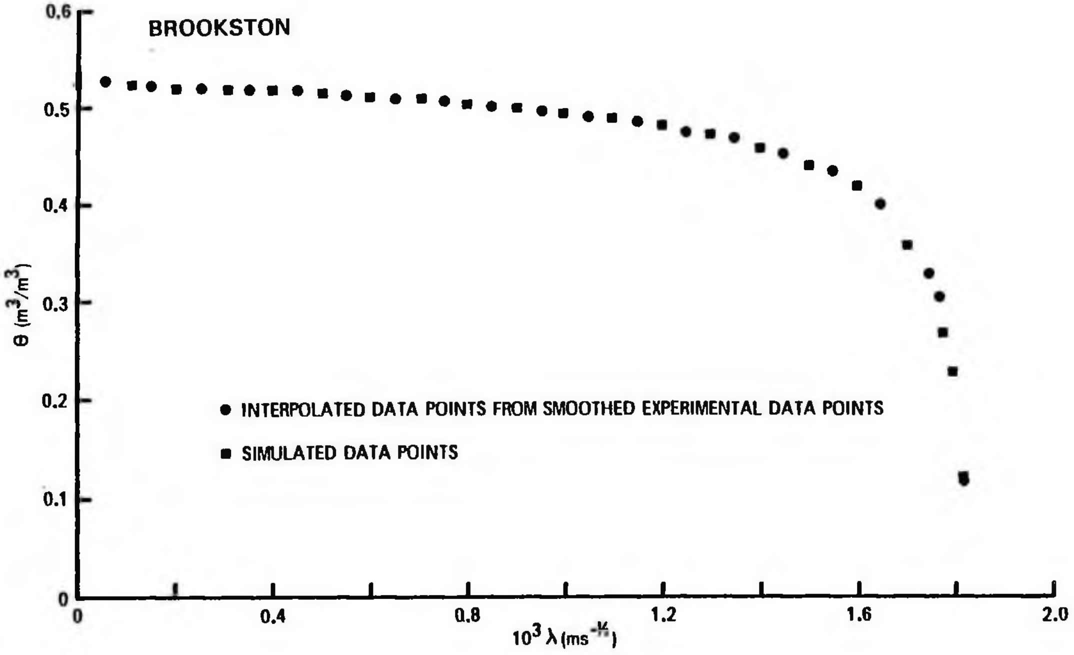

BROOKSTON
0.6
0.5
0.4
0.3
0.2
0.1
0
θ (m³/m³)
0
0.4
0.8
1.2
1.6
2.0
10³ λ (ms⁻½)
● INTERPOLATED DATA POINTS FROM SMOOTHED EXPERIMENTAL DATA POINTS
■ SIMULATED DATA POINTS

Figure 5.16b

TABLE 5.5a. Computer output for soil moisture diffusivity D, experimentally determined water content THLA and simulated water content THETA2. THETA1 is the integration of $d\theta/d\lambda$ (which was done with the DERIV algorithm of CSMP) to serve as a check on the accuracy of DERIV algorithm of CSMP (Akuse clay).

```
CALCULATION OF SOIL MOISTURE DIFFUSIVITY AND SIMULATION OF                DKS        INTEGRATION
WATER CONTENT AS A FUNCTION OF LAMBDA. (AKUSE CLAY)

  LAMBDA         G            THETAA         D             THETA1         THLA           THETA2
 0.0          1.7491E-03   5.2600E-01   8.7453E-05   5.2600E-01   5.2600E-01   5.2600E-01
 9.1200E-05   1.7490E-03   5.2509E-01   8.7519E-05   5.2509E-01   5.2509E-01   5.2509E-01
 1.8240E-04   1.7489E-03   5.2418E-01   8.7293E-05   5.2418E-01   5.2418E-01   5.2418E-01
 2.7360E-04   1.7487E-03   5.2327E-01   8.7496E-05   5.2327E-01   5.2326E-01   5.2327E-01
 3.6480E-04   1.7484E-03   5.2236E-01   8.7435E-05   5.2236E-01   5.2235E-01   5.2236E-01
 4.5600E-04   1.7480E-03   5.2144E-01   8.7463E-05   5.2145E-01   5.2144E-01   5.2144E-01
 5.4720E-04   1.7476E-03   5.2053E-01   8.7361E-05   5.2053E-01   5.2053E-01   5.2053E-01
 6.3840E-04   1.7470E-03   5.1963E-01   9.1608E-05   5.1963E-01   5.1964E-01   5.1963E-01
 7.2960E-04   1.7465E-03   5.1881E-01   9.9960E-05   5.1881E-01   5.1882E-01   5.1881E-01
 8.2080E-04   1.7459E-03   5.1801E-01   1.0157E-04   5.1801E-01   5.1802E-01   5.1801E-01
 9.1200E-04   1.7452E-03   5.1724E-01   1.0520E-04   5.1724E-01   5.1725E-01   5.1724E-01
 1.0032E-03   1.7445E-03   5.1650E-01   1.0922E-04   5.1650E-01   5.1651E-01   5.1650E-01
 1.0944E-03   1.7437E-03   5.1578E-01   1.1352E-04   5.1579E-01   5.1579E-01   5.1578E-01
 1.1856E-03   1.7429E-03   5.1509E-01   1.1800E-04   5.1510E-01   5.1511E-01   5.1510E-01
 1.2768E-03   1.7420E-03   5.1437E-01   1.0243E-04   5.1436E-01   5.1436E-01   5.1436E-01
 1.3680E-03   1.7410E-03   5.1359E-01   1.0357E-04   5.1360E-01   5.1360E-01   5.1359E-01
 1.4592E-03   1.7399E-03   5.1283E-01   1.0446E-04   5.1284E-01   5.1284E-01   5.1283E-01
 1.5504E-03   1.7388E-03   5.1207E-01   1.0430E-04   5.1208E-01   5.1208E-01   5.1207E-01
 1.6416E-03   1.7376E-03   5.1131E-01   1.0430E-04   5.1132E-01   5.1132E-01   5.1131E-01
 1.7328E-03   1.7363E-03   5.1055E-01   1.0430E-04   5.1056E-01   5.1056E-01   5.1055E-01
 1.8240E-03   1.7348E-03   5.0978E-01   9.2723E-05   5.0979E-01   5.0974E-01   5.0974E-01
 1.9152E-03   1.7329E-03   5.0871E-01   6.8692E-05   5.0871E-01   5.0870E-01   5.0871E-01
 2.0064E-03   1.7307E-03   5.0759E-01   6.8966E-05   5.0760E-01   5.0759E-01   5.0759E-01
 2.0976E-03   1.7283E-03   5.0641E-01   6.4896E-05   5.0642E-01   5.0641E-01   5.0641E-01
 2.1888E-03   1.7256E-03   5.0516E-01   6.1330E-05   5.0517E-01   5.0516E-01   5.0516E-01
 2.2800E-03   1.7241E-03   5.0444E-01   2.0026E-04   5.0445E-01   5.0448E-01   5.0444E-01
 2.3712E-03   1.7232E-03   5.0407E-01   2.0505E-04   5.0416E-01   5.0419E-01   5.0417E-01
 2.4624E-03   1.7216E-03   5.0360E-01   9.7851E-05   5.0361E-01   5.0341E-01   5.0360E-01
 2.5536E-03   1.7171E-03   5.0215E-01   3.3643E-05   5.0216E-01   5.0164E-01   5.0215E-01
 2.6448E-03   1.7100E-03   4.9883E-01   2.3999E-05   4.9884E-01   4.9888E-01   4.9883E-01
 2.7360E-03   1.7050E-03   4.9700E-01   5.6314E-05   4.9701E-01   4.9704E-01   4.9700E-01
 2.8272E-03   1.7015E-03   4.9575E-01   8.0298E-05   4.9577E-01   4.9579E-01   4.9576E-01
 2.9184E-03   1.6996E-03   4.9608E-01   2.0179E-04   4.9619E-01   4.9511E-01   4.9604E-01
 3.0096E-03   1.6984E-03   4.9495E-01   3.0560E-04   4.9496E-01   4.9472E-01   4.9495E-01
 3.1008E-03   1.6890E-03   4.9175E-01   2.2473E-05   4.9177E-01   4.9164E-01   4.9176E-01
 3.1920E-03   1.6771E-03   4.8798E-01   1.8563E-05   4.8800E-01   4.8736E-01   4.8798E-01
 3.2832E-03   1.6658E-03   4.8443E-01   2.2743E-05   4.8445E-01   4.8438E-01   4.8443E-01
 3.3744E-03   1.6545E-03   4.8103E-01   2.2269E-05   4.8105E-01   4.8096E-01   4.8103E-01
 3.4656E-03   1.6403E-03   4.7716E-01   1.6588E-05   4.7719E-01   4.7681E-01   4.7717E-01
 3.5568E-03   1.6239E-03   4.7228E-01   1.5090E-05   4.7231E-01   4.7216E-01   4.7229E-01
 3.6480E-03   1.6062E-03   4.6757E-01   1.4515E-05   4.6760E-01   4.6724E-01   4.6757E-01
 3.7392E-03   1.5825E-03   4.6150E-01   1.0071E-05   4.6154E-01   4.6083E-01   4.6150E-01
 3.8304E-03   1.5512E-03   4.5253E-01   7.6931E-06   4.5259E-01   4.5256E-01   4.5254E-01
 3.9216E-03   1.5227E-03   4.4568E-01   5.2453E-06   4.4574E-01   4.4522E-01   4.4569E-01
 4.0128E-03   1.4751E-03   4.3338E-01   4.5015E-06   4.3345E-01   4.3322E-01   4.3334E-01
 4.1040E-03   1.4186E-03   4.1966E-01   4.4214E-06   4.1975E-01   4.1930E-01   4.1967E-01
 4.1952E-03   1.3429E-03   4.0149E-01   3.0061E-06   4.0161E-01   4.0107E-01   4.0150E-01
 4.2864E-03   1.2309E-03   3.7540E-01   1.8404E-06   3.7558E-01   3.7467E-01   3.7541E-01
 4.3776E-03   1.0799E-03   3.4044E-01   1.2609E-06   3.4072E-01   3.3983E-01   3.4046E-01
 4.4688E-03   8.4410E-04   2.8715E-01   3.9825E-07   2.8756E-01   2.8659E-01   2.8717E-01
 4.5600E-03  -2.1653E-08   9.9961E-02  -3.2569E-12   1.0293E-01   1.0011E-01   1.0000E-01
```

TABLE 5.5b. Computer output for soil moisture diffusivity D, experimental water content THLA and simulated water content THETA2. THETA1 is the integration of $d\theta/d\lambda$ to serve as a check on the accuracy of the DERIV algorithm of CSMP (Brookston clay).

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CALCULATION OF SOIL MOISTURE DIFFUSIVITY AND SIMULATION OF              RKS       INTEGRATION
WATER CONTENT AS A FUNCTION OF LAMBDA. (BROOKSTON CLAY)

  LAMBDA       G           THETAA      D           THETA1      THLA        THETA2
  0.0          6.5185E-04  5.3000E-01  6.5185E-05  5.3000E-01  5.3000E-01  5.3000E-01
  3.6400E-05   6.5182E-04  5.2818E-01  6.5284E-06  5.2818E-01  5.2818E-01  5.2818E-01
  7.2800E-05   6.5172E-04  5.2636E-01  6.5156E-06  5.2636E-01  5.2634E-01  5.2636E-01
  1.0920E-04   6.5156E-04  5.2455E-01  6.9937E-06  5.2455E-01  5.2462E-01  5.2455E-01
  1.4560E-04   6.5139E-04  5.2323E-01  1.0248E-05  5.2324E-01  5.2327E-01  5.2323E-01
  1.8200E-04   6.5120E-04  5.2210E-01  1.1627E-05  5.2211E-01  5.2214E-01  5.2210E-01
  2.1840E-04   6.5102E-04  5.2119E-01  1.4841E-05  5.2120E-01  5.2123E-01  5.2119E-01
  2.5480E-04   6.5086E-04  5.2051E-01  2.0515E-05  5.2052E-01  5.2055E-01  5.2051E-01
  2.9120E-04   6.5073E-04  5.2004E-01  3.3211E-05  5.2005E-01  5.2008E-01  5.2004E-01
  3.2760E-04   6.5049E-04  5.1943E-01  1.2835E-05  5.1944E-01  5.1931E-01  5.1943E-01
  3.6400E-04   6.5018E-04  5.1848E-01  1.2070E-05  5.1849E-01  5.1840E-01  5.1848E-01
  4.0040E-04   6.4983E-04  5.1756E-01  1.3001E-05  5.1758E-01  5.1749E-01  5.1756E-01
  4.3680E-04   6.4945E-04  5.1665E-01  1.2987E-05  5.1667E-01  5.1658E-01  5.1665E-01
  4.7320E-04   6.4904E-04  5.1574E-01  1.2977E-05  5.1576E-01  5.1567E-01  5.1574E-01
  5.0960E-04   6.4859E-04  5.1483E-01  1.2970E-05  5.1485E-01  5.1476E-01  5.1483E-01
  5.4600E-04   6.4811E-04  5.1392E-01  1.2958E-05  5.1394E-01  5.1385E-01  5.1392E-01
  5.8240E-04   6.4760E-04  5.1301E-01  1.2954E-05  5.1303E-01  5.1294E-01  5.1301E-01
  6.1880E-04   6.4705E-04  5.1210E-01  1.2939E-05  5.1212E-01  5.1203E-01  5.1210E-01
  6.5520E-04   6.4647E-04  5.1119E-01  1.2925E-05  5.1121E-01  5.1112E-01  5.1119E-01
  6.9160E-04   6.4586E-04  5.1028E-01  1.2921E-05  5.1030E-01  5.1021E-01  5.1028E-01
  7.2800E-04   6.4493E-04  5.0908E-01  7.7768E-06  5.0911E-01  5.0897E-01  5.0908E-01
  7.6440E-04   6.4375E-04  5.0747E-01  6.8581E-06  5.0750E-01  5.0733E-01  5.0747E-01
  8.0080E-04   6.4239E-04  5.0573E-01  6.4109E-06  5.0576E-01  5.0558E-01  5.0573E-01
  8.3720E-04   6.4083E-04  5.0382E-01  5.8623E-06  5.0385E-01  5.0368E-01  5.0382E-01
  8.7360E-04   6.3905E-04  5.0174E-01  5.3975E-06  5.0178E-01  5.0161E-01  5.0175E-01
  9.1000E-04   6.3718E-04  4.9953E-01  5.4594E-06  4.9957E-01  4.9950E-01  4.9953E-01
  9.4640E-04   6.3549E-04  4.9777E-01  6.8969E-06  4.9781E-01  4.9766E-01  4.9777E-01
  9.8280E-04   6.3373E-04  4.9596E-01  6.3368E-06  4.9600E-01  4.9586E-01  4.9596E-01
  1.0192E-03   6.3191E-04  4.9413E-01  6.3171E-06  4.9418E-01  4.9404E-01  4.9414E-01
  1.0556E-03   6.3002E-04  4.9231E-01  6.3007E-06  4.9236E-01  4.9222E-01  4.9232E-01
  1.0920E-03   6.2807E-04  4.9049E-01  6.2797E-06  4.9054E-01  4.9040E-01  4.9049E-01
  1.1284E-03   6.2503E-04  4.8802E-01  3.5687E-06  4.8807E-01  4.8767E-01  4.8802E-01
  1.1648E-03   6.2093E-04  4.8438E-01  2.8242E-06  4.8444E-01  4.8409E-01  4.8439E-01
  1.2012E-03   6.1597E-04  4.8013E-01  2.4916E-06  4.8020E-01  4.7990E-01  4.8014E-01
  1.2376E-03   6.1245E-04  4.7741E-01  5.0050E-06  4.7748E-01  4.7702E-01  4.7742E-01
  1.2740E-03   6.0934E-04  4.7496E-01  4.8613E-06  4.7504E-01  4.7453E-01  4.7496E-01
  1.3104E-03   6.0619E-04  4.7280E-01  4.5872E-06  4.7288E-01  4.7210E-01  4.7280E-01
  1.3468E-03   6.0166E-04  4.6927E-01  2.8125E-06  4.6936E-01  4.6869E-01  4.6928E-01
  1.3832E-03   5.9647E-04  4.6540E-01  2.7121E-06  4.6554E-01  4.6489E-01  4.6544E-01
  1.4196E-03   5.8976E-04  4.6095E-01  2.0331E-06  4.6106E-01  4.6010E-01  4.6096E-01
  1.4560E-03   5.8084E-04  4.5466E-01  1.5317E-06  4.5479E-01  4.5391E-01  4.5467E-01
  1.4924E-03   5.7014E-04  4.4737E-01  1.3326E-06  4.4752E-01  4.4665E-01  4.4738E-01
  1.5288E-03   5.5908E-04  4.3976E-01  1.3819E-06  4.3993E-01  4.3932E-01  4.3977E-01
  1.5652E-03   5.4614E-04  4.3200E-01  1.1212E-06  4.3219E-01  4.3097E-01  4.3201E-01
  1.6016E-03   5.2788E-04  4.2038E-01  7.3224E-07  4.2061E-01  4.1944E-01  4.2039E-01
  1.6380E-03   5.0490E-04  4.0612E-01  5.9260E-07  4.0641E-01  4.0526E-01  4.0614E-01
  1.6744E-03   4.7399E-04  3.8819E-01  4.1317E-07  3.8856E-01  3.8661E-01  3.8821E-01
  1.7108E-03   4.3155E-04  3.6342E-01  2.7787E-07  3.6395E-01  3.6155E-01  3.6344E-01
  1.7472E-03   3.7338E-04  3.2943E-01  1.7920E-07  3.3024E-01  3.2792E-01  3.2945E-01
  1.7836E-03   2.7597E-04  2.7567E-01  7.6241E-08  2.7716E-01  2.7279E-01  2.7569E-01
  1.8200E-03   1.3737E-08  1.1996E-01  9.4712E-13  1.2468E-01  1.2000E-01  1.2003E-01
```

FIGURE 5.17.

(a) Simulated chloride content as a function of λ. Interpolated experimental data points are provided for comparison (Akuse clay).

(b) Simulated chloride content as a function of λ (Brookston clay).

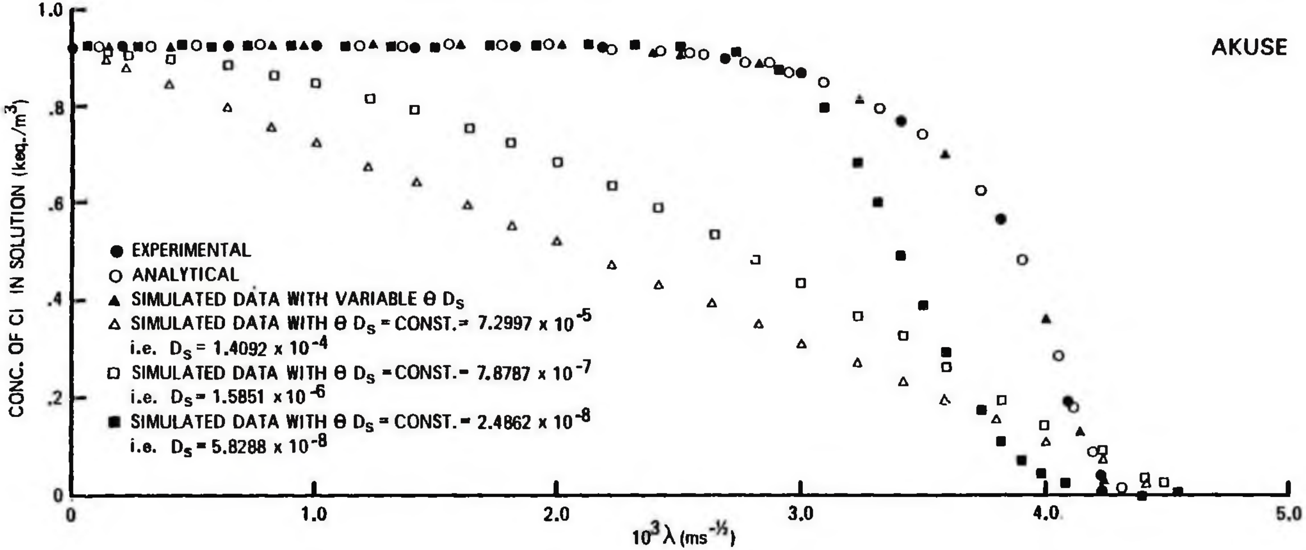
AKUSE
1.0
.8
.6
.4
.2
0
CONC. OF Cl IN SOLUTION (keq./m^3)
0
1.0
2.0
3.0
4.0
5.0
$10^3 \lambda$ (ms$^{-½}$)
● EXPERIMENTAL
○ ANALYTICAL
▲ SIMULATED DATA WITH VARIABLE θ D_S
△ SIMULATED DATA WITH θ D_S = CONST.= 7.2997×10^{-5}
i.e. $D_S = 1.4092 \times 10^{-4}$
☐ SIMULATED DATA WITH θ D_S = CONST.= 7.8787×10^{-7}
i.e. $D_S = 1.5851 \times 10^{-6}$
■ SIMULATED DATA WITH θ D_S = CONST.= 2.4862×10^{-8}
i.e. $D_S = 5.8288 \times 10^{-8}$

Figure 5.17a

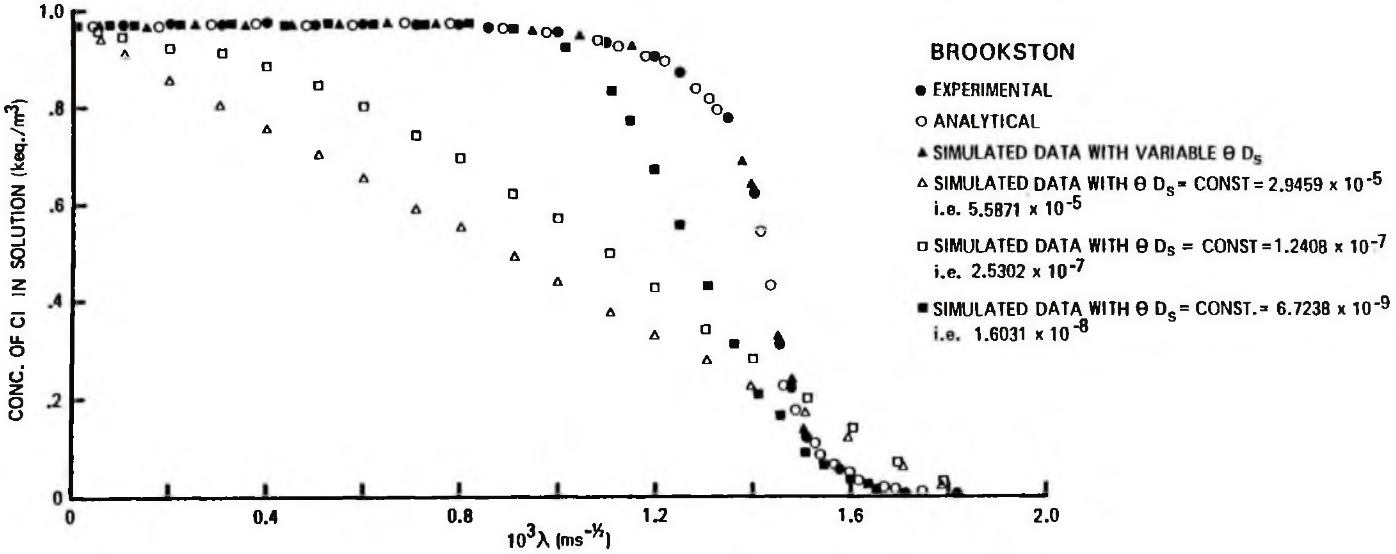
1.0
.8
.6
.4
.2
0
CONC. OF Cl IN SOLUTION (keq./m³)
0
0.4
0.8
1.2
1.6
2.0
10³λ (ms^-½)
BROOKSTON
● EXPERIMENTAL
○ ANALYTICAL
▲ SIMULATED DATA WITH VARIABLE θ Ds
△ SIMULATED DATA WITH θ Ds = CONST = 2.9459 x 10^-5 i.e. 5.5871 x 10^-5
□ SIMULATED DATA WITH θ Ds = CONST = 1.2408 x 10^-7 i.e. 2.5302 x 10^-7
■ SIMULATED DATA WITH θ Ds = CONST. = 6.7238 x 10^-9 i.e. 1.6031 x 10^-8

Figure 5.17b

TABLE 5.6a. Computer output showing experimental $c(\lambda)$, $c(\lambda)$ from analytical solution (equation 3.21) and $c(\lambda)$ simulated non-analytically using the algorithm in Appendix D (Akuse clay).

DISPERSION - ANALYTICAL AND NON-ANALYTICAL SOLUTIONS(AKUSE) SIMP INTEGRATION

LAMDA	THLA	D	THDS	DS	AH	SEELA	SEE1	SEE2
0.0	5.2600E-01	8.7448E-05	7.1818E-05	1.3654E-04	-2.4353E 01	9.2000E-01	9.2000E-01	9.2000E-01
9.1200E-05	5.2509E-01	8.8273E-05	6.7668E-05	1.2887E-04	-2.5138E 01	9.1991E-01	9.1991E-01	9.1991E-01
1.8240E-04	5.2418E-01	8.8232E-05	6.3978E-05	1.2205E-04	-2.5840E 01	9.1982E-01	9.1982E-01	9.1981E-01
2.7360E-04	5.2326E-01	8.7123E-05	6.7812E-05	1.2959E-04	-2.3675E 01	9.1973E-01	9.1972E-01	9.1972E-01
3.6480E-04	5.2235E-01	8.6872E-05	5.7700E-05	1.1046E-04	-2.6997E 01	9.1963E-01	9.1963E-01	9.1963E-01
4.5600E-04	5.2144E-01	8.7022E-05	6.4175E-05	1.2307E-04	-2.3532E 01	9.1954E-01	9.1953E-01	9.1953E-01
5.4720E-04	5.2053E-01	8.5699E-05	5.5061E-05	1.0578E-04	-2.6564E 01	9.1945E-01	9.1944E-01	9.1944E-01
6.3840E-04	5.1964E-01	9.4910E-05	5.7867E-05	1.1136E-04	-2.4456E 01	9.1936E-01	9.1935E-01	9.1934E-01
7.2960E-04	5.1882E-01	9.8431E-05	6.8141E-05	1.3134E-04	-2.0074E 01	9.1927E-01	9.1925E-01	9.1925E-01
8.2080E-04	5.1802E-01	1.0302E-04	6.8202E-05	1.3166E-04	-1.9363E 01	9.1918E-01	9.1916E-01	9.1915E-01
9.1200E-04	5.1725E-01	1.0443E-04	5.8021E-05	1.1217E-04	-2.1947E 01	9.1909E-01	9.1906E-01	9.1906E-01
1.0032E-03	5.1651E-01	1.0994E-04	6.4519E-05	1.2491E-04	-1.9006E 01	9.1900E-01	9.1897E-01	9.1896E-01
1.0944E-03	5.1579E-01	1.1451E-04	6.8367E-05	1.3255E-04	-1.7248E 01	9.1891E-01	9.1888E-01	9.1887E-01
1.1856E-03	5.1511E-01	1.1917E-04	6.4618E-05	1.2545E-04	-1.7521E 01	9.1881E-01	9.1878E-01	9.1877E-01
1.2768E-03	5.1436E-01	1.0419E-04	6.4665E-05	1.2572E-04	-1.6782E 01	9.1872E-01	9.1868E-01	9.1868E-01
1.3680E-03	5.1360E-01	1.0360E-04	6.8515E-05	1.3340E-04	-1.5155E 01	9.1863E-01	9.1859E-01	9.1858E-01
1.4592E-03	5.1284E-01	1.0485E-04	6.1343E-05	1.1961E-04	-1.6164E 01	9.1854E-01	9.1850E-01	9.1849E-01
1.5504E-03	5.1208E-01	1.0414E-04	6.4792E-05	1.2653E-04	-1.4582E 01	9.1845E-01	9.1840E-01	9.1840E-01
1.6416E-03	5.1132E-01	1.0432E-04	7.2935E-05	1.4264E-04	-1.2314E 01	9.1836E-01	9.1831E-01	9.1830E-01
1.7328E-03	5.1056E-01	1.0404E-04	6.4866E-05	1.2705E-04	-1.3128E 01	9.1827E-01	9.1822E-01	9.1821E-01
1.8240E-03	5.0974E-01	7.9789E-05	5.8411E-05	1.1459E-04	-1.3782E 01	9.1818E-01	9.1812E-01	9.1811E-01
1.9152E-03	5.0870E-01	7.2937E-05	6.1516E-05	1.2093E-04	-1.2331E 01	9.1808E-01	9.1803E-01	9.1802E-01
2.0064E-03	5.0759E-01	6.9465E-05	5.5684E-05	1.0970E-04	-1.2791E 01	9.1799E-01	9.1793E-01	9.1792E-01
2.0976E-03	5.0641E-01	6.5082E-05	6.8815E-05	1.3589E-04	-9.6781E 00	9.1790E-01	9.1784E-01	9.1783E-01
2.1888E-03	5.0516E-01	6.1082E-05	6.8694E-07	1.3598E-06	-9.0238E 02	9.1127E-01	9.1126E-01	9.1125E-01
2.2800E-03	5.0448E-01	1.5662E-04	2.3655E-06	4.6890E-06	-2.4259E 02	9.0627E-01	9.0623E-01	9.0622E-01
2.3712E-03	5.0408E-01	2.6446E-04	-3.0854E-04	-6.1207E-04	1.7108E 00	9.0483E-01	9.0479E-01	9.0478E-01
2.4624E-03	5.0341E-01	8.2375E-05	3.0841E-06	6.1264E-06	-1.5626E 02	9.0344E-01	9.0336E-01	9.0335E-01
2.5536E-03	5.0164E-01	2.7959E-05	3.0896E-06	6.1591E-06	-1.4114E 02	9.0116E-01	9.0107E-01	9.0106E-01
2.6448E-03	4.9888E-01	3.6624E-05	8.1005E-07	1.6237E-06	-4.8201E 02	8.9614E-01	8.9607E-01	8.9605E-01
2.7360E-03	4.9704E-01	5.0008E-05	8.0627E-07	1.6221E-06	-4.2795E 02	8.8640E-01	8.8630E-01	8.8628E-01
2.8272E-03	4.9579E-01	8.0216E-05	8.2248E-07	1.6589E-06	-3.6448E 02	8.7728E-01	8.7718E-01	8.7716E-01
2.9184E-03	4.9511E-01	2.0503E-04	8.3459E-07	1.6857E-06	-3.0506E 02	8.6816E-01	8.6806E-01	8.6804E-01
3.0096E-03	4.9472E-01	2.8232E-05	5.3072E-07	1.0728E-06	-3.9467E 02	8.5851E-01	8.5836E-01	8.5834E-01
3.1008E-03	4.9164E-01	2.2482E-05	3.6261E-07	7.3756E-07	-4.5359E 02	8.3984E-01	8.3966E-01	8.3963E-01
3.1920E-03	4.8786E-01	1.8557E-05	4.3840E-07	8.9862E-07	-2.7329E 02	8.2160E-01	8.2146E-01	8.2144E-01
3.2832E-03	4.8438E-01	2.2231E-05	4.4271E-07	9.1398E-07	-1.7049E 02	8.0336E-01	8.0323E-01	8.0320E-01
3.3744E-03	4.8096E-01	2.2080E-05	2.7494E-07	5.7165E-07	-1.1444E 02	7.7863E-01	7.7856E-01	7.7853E-01
3.4656E-03	4.7681E-01	1.5974E-05	2.4971E-07	5.2371E-07	4.8939E 01	7.4760E-01	7.4752E-01	7.4749E-01
3.5568E-03	4.7216E-01	1.6240E-05	2.2007E-07	4.6609E-07	2.5215E 02	7.1289E-01	7.1282E-01	7.1278E-01
3.6480E-03	4.6724E-01	1.3462E-05	1.7513E-07	3.7481E-07	5.6149E 02	6.7225E-01	6.7215E-01	6.7211E-01
3.7392E-03	4.6083E-01	9.1142E-06	1.4294E-07	3.1018E-07	9.8415E 02	6.2267E-01	6.2258E-01	6.2254E-01
3.8304E-03	4.5256E-01	9.9514E-06	9.8974E-08	2.1870E-07	1.8420E 03	5.6181E-01	5.6177E-01	5.6171E-01
3.9216E-03	4.4522E-01	6.8695E-06	6.4184E-08	1.4416E-07	3.4786E 03	4.7704E-01	4.7708E-01	4.7701E-01
4.0128E-03	4.3322E-01	5.2440E-06	3.5752E-08	8.2527E-08	7.3659E 03	3.6031E-01	3.6043E-01	3.6035E-01
4.1040E-03	4.1930E-01	3.9449E-06	2.3239E-08	5.5425E-08	1.3005E 04	1.9384E-01	1.9385E-01	1.9378E-01
4.1952E-03	4.0107E-01	3.0170E-06	2.5497E-08	6.3573E-08	1.3322E 04	7.7232E-02	7.7514E-02	7.7469E-02
4.2864E-03	3.7467E-01	1.8300E-06	1.3649E-08	3.6430E-08	2.7483E 04	1.7856E-02	1.7820E-02	1.7820E-02
4.3776E-03	3.3983E-01	1.2628E-06	1.2973E-08	3.8175E-08	3.1431E 04	6.2403E-03	6.2461E-03	6.2371E-03
4.4688E-03	2.8659E-01	4.1189E-07	8.8302E-09	3.0811E-08	4.9445E 04	6.0000E-04	6.0701E-04	6.0236E-04
4.5600E-03	1.0000E-01	0.0	0.0	0.0	8.3507E 05	6.0000E-05	6.2644E-05	5.9440E-05

TABLE 5.6b. Computer output showing experimental c(λ), c(λ) from analytical solution (equation 3.21) and computer solution for c(λ) using the algorithm in Appendix D (Brookston clay).

```
DISPERSION - ANALYTICAL AND NON-ANALYTICAL SOLUTIONS(BROOKSTON)        SIMP     INTEGRATION

  LAMDA         THLA          D             THDS          DS            AH             SEELA         SEE1          SEE2
 0.0          5.3000E-01    6.5182E-05    2.6738E-05    5.0449E-05    -2.4378E 01    9.7000E-01    9.7000E-01    9.7000E-01
 3.6400E-05   5.2818E-01    6.5210E-06    2.3778E-05    4.5019E-05    -2.6603E 01    9.6996E-01    9.6996E-01    9.6996E-01
 7.2800E-05   5.2636E-01    6.5205E-06    2.5188E-05    4.7853E-05    -2.4352E 01    9.6993E-01    9.6992E-01    9.6992E-01
 1.0920E-04   5.2462E-01    8.1046E-06    2.3799E-05    4.5364E-05    -2.4969E 01    9.6989E-01    9.6988E-01    9.6988E-01
 1.4560E-04   5.2327E-01    9.5646E-06    2.3809E-05    4.5500E-05    -2.4158E 01    9.6985E-01    9.6985E-01    9.6985E-01
 1.8200E-04   5.2214E-01    1.1657E-05    2.2565E-05    4.3216E-05    -2.4647E 01    9.6982E-01    9.6981E-01    9.6981E-01
 2.1840E-04   5.2123E-01    1.4848E-05    2.3828E-05    4.5714E-05    -2.2543E 01    9.6978E-01    9.6977E-01    9.6977E-01
 2.5480E-04   5.2055E-01    2.0359E-05    2.0432E-05    3.9251E-05    -2.5362E 01    9.6975E-01    9.6973E-01    9.6973E-01
 2.9120E-04   5.2008E-01    3.3263E-05    2.3846E-05    4.5851E-05    -2.0937E 01    9.6971E-01    9.6969E-01    9.6969E-01
 3.2760E-04   5.1931E-01    1.2907E-05    2.2599E-05    4.3518E-05    -2.1255E 01    9.6967E-01    9.6965E-01    9.6965E-01
 3.6400E-04   5.1840E-01    1.2961E-05    2.1477E-05    4.1430E-05    -2.1486E 01    9.6964E-01    9.6961E-01    9.6961E-01
 4.0040E-04   5.1749E-01    1.2919E-05    2.2615E-05    4.3701E-05    -1.9571E 01    9.6960E-01    9.6957E-01    9.6957E-01
 4.3680E-04   5.1658E-01    1.2972E-05    2.2622E-05    4.3793E-05    -1.8733E 01    9.6956E-01    9.6953E-01    9.6953E-01
 4.7320E-04   5.1567E-01    1.2916E-05    2.0474E-05    3.9704E-05    -1.9781E 01    9.6953E-01    9.6949E-01    9.6949E-01
 5.0960E-04   5.1476E-01    1.2871E-05    2.3893E-05    4.6416E-05    -1.6165E 01    9.6949E-01    9.6945E-01    9.6945E-01
 5.4600E-04   5.1385E-01    1.2929E-05    1.9555E-05    3.8055E-05    -1.8795E 01    9.6945E-01    9.6941E-01    9.6941E-01
 5.8240E-04   5.1294E-01    1.2949E-05    2.8688E-05    5.5928E-05    -1.2160E 01    9.6942E-01    9.6937E-01    9.6937E-01
 6.1880E-04   5.1203E-01    1.2914E-05    2.0496E-05    4.0030E-05    -1.6109E 01    9.6938E-01    9.6933E-01    9.6933E-01
 6.5520E-04   5.1112E-01    1.2903E-05    2.0501E-05    4.0111E-05    -1.5197E 01    9.6934E-01    9.6929E-01    9.6929E-01
 6.9160E-04   5.1021E-01    1.2866E-05    2.1531E-05    4.2200E-05    -1.3607E 01    9.6931E-01    9.6925E-01    9.6925E-01
 7.2800E-04   5.0890E-01    7.8572E-06    2.2669E-05    4.4545E-05    -1.2106E 01    9.6927E-01    9.6921E-01    9.6921E-01
 7.6440E-04   5.0733E-01    7.0510E-06    1.9582E-05    3.8598E-05    -1.3070E 01    9.6924E-01    9.6917E-01    9.6917E-01
 8.0080E-04   5.0558E-01    6.4002E-06    2.0041E-06    3.9640E-06    -1.1850E 02    9.6916E-01    9.6913E-01    9.6912E-01
 8.3720E-04   5.0368E-01    5.8509E-06    3.3788E-07    6.7083E-07    -6.4854E 02    9.6684E-01    9.6676E-01    9.6676E-01
 8.7360E-04   5.0161E-01    5.3988E-06    2.4237E-07    4.8319E-07    -8.2863E 02    9.6331E-01    9.6324E-01    9.6324E-01
 9.1000E-04   4.9950E-01    6.3716E-06    2.8845E-07    5.7748E-07    -6.3309E 02    9.5904E-01    9.5897E-01    9.5897E-01
 9.4640E-04   4.9768E-01    6.3438E-06    2.8273E-07    5.6810E-07    -5.8172E 02    9.5546E-01    9.5539E-01    9.5540E-01
 9.8280E-04   4.9586E-01    6.3451E-06    2.7745E-07    5.5952E-07    -5.2762E 02    9.5178E-01    9.5171E-01    9.5172E-01
 1.0192E-03   4.9404E-01    6.3140E-06    1.7061E-07    3.4533E-07    -7.5244E 02    9.4694E-01    9.4687E-01    9.4688E-01
 1.0556E-03   4.9222E-01    6.2824E-06    1.4247E-07    2.8945E-07    -7.7504E 02    9.4011E-01    9.4006E-01    9.4007E-01
 1.0920E-03   4.9040E-01    6.2644E-06    1.2268E-07    2.5016E-07    -7.5433E 02    9.3197E-01    9.3192E-01    9.3193E-01
 1.1284E-03   4.8767E-01    3.4965E-06    9.4875E-08    1.9455E-07    -7.8772E 02    9.2159E-01    9.2155E-01    9.2157E-01
 1.1648E-03   4.8409E-01    2.8899E-06    8.2110E-08    1.6962E-07    -6.9478E 02    9.0903E-01    9.0901E-01    9.0904E-01
 1.2012E-03   4.7990E-01    2.8060E-06    7.0756E-08    1.4744E-07    -5.5831E 02    8.9446E-01    8.9448E-01    8.9451E-01
 1.2376E-03   4.7702E-01    4.1544E-06    5.9358E-08    1.2444E-07    -3.7215E 02    8.7667E-01    8.7669E-01    8.7673E-01
 1.2740E-03   4.7453E-01    4.8452E-06    3.5140E-08    7.4052E-08    -1.3585E 02    8.5090E-01    8.5099E-01    8.5105E-01
 1.3104E-03   4.7210E-01    3.4430E-06    2.8114E-08    5.9551E-08     4.4309E 02    8.1376E-01    8.1389E-01    8.1397E-01
 1.3468E-03   4.6869E-01    3.0381E-06    2.3142E-08    4.9376E-08     1.2782E 03    7.6929E-01    7.6948E-01    7.6959E-01
 1.3832E-03   4.6489E-01    2.7121E-06    1.0780E-08    2.3188E-08     4.3201E 03    6.8925E-01    6.8972E-01    6.8988E-01
 1.4196E-03   4.6010E-01    1.8924E-06    4.4195E-09    9.6054E-09     1.4348E 04    5.4228E-01    5.4337E-01    5.4363E-01
 1.4560E-03   4.5391E-01    1.5717E-06    3.1245E-09    6.8835E-09     2.5620E 04    3.2000E-01    3.1882E-01    3.1934E-01
 1.4924E-03   4.4665E-01    1.3324E-06    6.2260E-09    1.3939E-08     1.5490E 04    1.7371E-01    1.7473E-01    1.7547E-01
 1.5288E-03   4.3932E-01    1.3903E-06    4.7673E-09    1.0851E-08     2.3611E 04    1.0680E-01    1.0600E-01    1.0683E-01
 1.5652E-03   4.3097E-01    9.7335E-07    5.4237E-09    1.2585E-08     2.3676E 04    6.9800E-02    6.8655E-02    6.9539E-02
 1.6016E-03   4.1944E-01    7.4715E-07    7.0499E-09    1.6808E-08     2.0411E 04    4.6279E-02    4.5221E-02    4.6139E-02
 1.6380E-03   4.0526E-01    5.9261E-07    7.3775E-09    1.8205E-08     2.1540E 04    2.6857E-02    2.5586E-02    2.6543E-02
 1.6744E-03   3.8661E-01    3.9659E-07    7.1151E-09    1.8404E-08     2.4363E 04    1.9079E-02    1.8033E-02    1.9000E-02
 1.7108E-03   3.6155E-01    2.6482E-07    7.0078E-09    1.9383E-08     2.6682E 04    1.3567E-02    1.2555E-02    1.3529E-02
 1.7472E-03   3.2792E-01    1.8070E-07    8.5612E-09    2.6108E-08     2.3309E 04    1.0170E-02    9.1612E-03    1.0139E-02
 1.7836E-03   2.7279E-01    6.6404E-08    3.4384E-09    1.2035E-08     6.1241E 04    7.3080E-03    6.3221E-03    7.3046E-03
 1.8200E-03   1.2000E-01    6.1019E-13    0.0           0.0           -4.8357E 07    5.0000E-03    3.9648E-03    5.0007E-03
```

Tables 5.6a and 5.6b, the experimental $c(\lambda)$ data, $c(\lambda)$ calculated from analytical solution and $c(\lambda)$ relationship simulated non-analytically are captioned SEELA, SEE1 and SEE2, respectively. The moisture content (THLA), moisture diffusivity (D), θD_s (THDS), D_s (DS) and $g/\theta D_s$ (AH) and $g = \theta\lambda - \int_{\theta_n}^{\theta} \lambda d\theta = \theta\lambda + 2D\frac{d\theta}{d\lambda}$) are also presented.

As observed in figures 5.17a, 5.17b, Tables 5.6a and 5.6b, agreement between the analytical solution, $c(\lambda)$ data simulated non-analytically with variable $D_s(\lambda)$ and experimental $c(\lambda)$ data is very good. Large deviations occur, however, when $c(\lambda)$ data is simulated using constant values of θD_s. For constant low value of $\theta D_s = 2.486 \times 10^{-8}\ m^2 s^{-1}$ (i.e. $D_s = 5.829 \times 10^{-8}\ m^2 s^{-1}$) the agreement with experimental $c(\lambda)$ data for Akuse clay is good up to $\lambda = 3.0 \times 10^{-3}\ ms^{-1/2}$, after which point substantial deviations occur. For Brookston clay the low θD_s value of $6.72 \times 10^{-9}\ m^2 s^{-1}$ (i.e. $D_s = 1.603 \times 10^{-8}\ m^2 s^{-1}$) shows good agreement with smoothed experimental data up to $\lambda = 1.0 \times 10^{-3}\ ms^{-1/2}$, after which deviations occur. It appears, therefore, that even though simulation using constant low value of θD_s predicts $c(\lambda)$ data similar to experimental $c(\lambda)$ from $\lambda=0$ until λ close to the wetting front, in general constant value of θD_s as was suggested by Smiles and Philip (1978) does not predict the $c(\lambda)$ relationship very well for the soils considered in this study.

Figures 5.18a and 5.18b present the simulated $c(\lambda)$ data for K^+ obtained from $D_s(\lambda)$ relationship derived from smoothed experimental $\theta(\lambda)$ and $c(\lambda)$ curves (figures 5.5a, 5.5c, 5.6a and 5.6c). Computer output for the data presented graphically in figures 5.18a and 5.18b are given in Tables 5.7a and 5.7b. Also printed in Tables 5.7a and 5.7b are the soil water diffusivity D, water content (THLA), $(\frac{g}{2}\frac{dc}{d\lambda} + \frac{\lambda\rho}{2}\frac{dS}{d\lambda})$ designated

FIGURE 5.18.

(a) Simulated K^+ content as a function of λ. Interpolated experimental data points are provided for comparison (Akuse clay).

(b) Simulated K^+ content as a function of λ (Brookston clay).

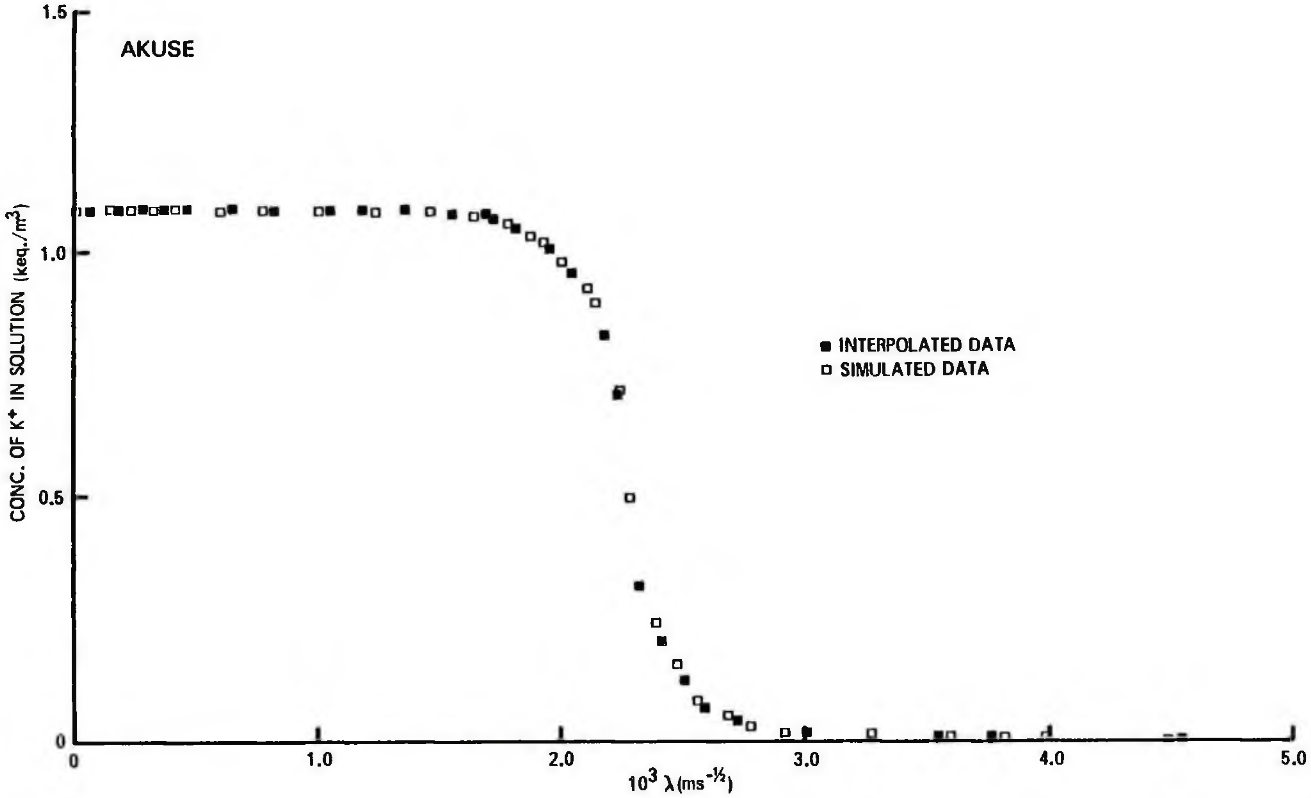
AKUSE
CONC. OF K⁺ IN SOLUTION (keq./m³)
1.5
1.0
0.5
0
0
1.0
2.0
3.0
4.0
5.0
10³ λ (ms⁻½)
■ INTERPOLATED DATA
□ SIMULATED DATA

Figure 5.18a

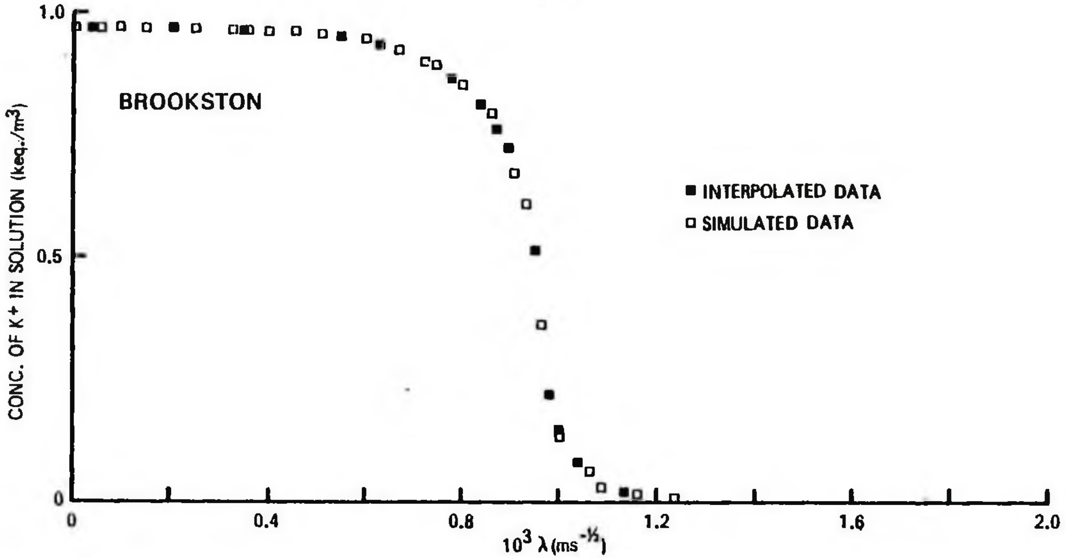
1.0
0.5
0
CONC. OF K+ IN SOLUTION (keq./m^3)
BROOKSTON
■ INTERPOLATED DATA
□ SIMULATED DATA
0
0.4
0.8
1.2
1.6
2.0
$10^3 \lambda\,(ms^{-1/2})$

Figure 5.18b

TABLE 5.7a. Computer output for simulation of concentration of K^+ in solution using calculated D_s values for Akuse clay.

```
DS FOR POTASSIUM AND SIMULATION OF CONCENTRATION (AKUSE CLAY)          RKS      INTEGRATION

 LAMBDA       D           E           THLA         LATHAD       THDS         DS           SEELA        SEE1
0.0         8.7453E-05 -4.5600E-04  5.2600E-01  2.1951E-04  2.2004E-04  4.1832E-04  1.0900E 00  1.0900E 00
9.1200E-05  8.7450E-05 -4.0811E-04  5.2509E-01  2.1238E-04  2.2014E-04  4.1925E-04  1.0900E 00  1.0900E 00
1.8240E-04  8.7425E-05 -3.6039E-04  5.2418E-01  2.0765E-04  2.1767E-04  4.1526E-04  1.0900E 00  1.0900E 00
2.7360E-04  8.7496E-05 -3.1283E-04  5.2326E-01  1.9733E-04  2.2115E-04  4.2263E-04  1.0899E 00  1.0899E 00
3.6480E-04  8.7435E-05 -2.6545E-04  5.2235E-01  1.9401E-04  2.1782E-04  4.1699E-04  1.0899E 00  1.0899E 00
4.5600E-04  8.7463E-05 -2.1822E-04  5.2144E-01  1.9476E-04  2.0828E-04  3.9943E-04  1.0899E 00  1.0899E 00
5.4720E-04  8.7361E-05 -1.7117E-04  5.2053E-01  1.6836E-04  2.3224E-04  4.4617E-04  1.0899E 00  1.0899E 00
6.3840E-04  9.1608E-05 -1.2426E-04  5.1964E-01  1.7554E-04  2.1471E-04  4.1319E-04  1.0898E 00  1.0898E 00
7.2960E-04  9.9960E-05 -7.7470E-05  5.1882E-01  1.5633E-04  2.2863E-04  4.4067E-04  1.0898E 00  1.0898E 00
8.2080E-04  1.0157E-04 -3.0809E-05  5.1802E-01  1.7467E-04  1.9971E-04  3.8552E-04  1.0898E 00  1.0898E 00
9.1200E-04  1.0520E-04  1.5732E-05  5.1725E-01  1.3714E-04  2.3638E-04  4.5699E-04  1.0898E 00  1.0898E 00
1.0032E-03  1.0922E-04  6.2160E-05  5.1651E-01  1.5013E-04  2.1174E-04  4.0994E-04  1.0897E 00  1.0897E 00
1.0944E-03  1.1352E-04  1.0848E-04  5.1579E-01  1.3573E-04  2.1830E-04  4.2323E-04  1.0897E 00  1.0897E 00
1.1856E-03  1.1800E-04  1.5471E-04  5.1511E-01  1.4024E-04  2.0276E-04  3.9362E-04  1.0897E 00  1.0897E 00
1.2768E-03  1.0243E-04  2.0073E-04  5.1436E-01  2.3713E-04  1.1449E-04  2.2260E-04  1.0897E 00  1.0896E 00
1.3680E-03  1.0357E-04  2.4660E-04  5.1360E-01  2.6727E-04  9.4688E-05  1.8436E-04  1.0896E 00  1.0896E 00
1.4592E-03  1.0446E-04  2.9234E-04  5.1284E-01  7.8975E-03  3.0449E-06  5.9373E-06  1.0885E 00  1.0885E 00
1.5504E-03  1.0430E-04  3.3793E-04  5.1208E-01  1.5258E-02  1.5066E-06  2.9422E-06  1.0858E 00  1.0862E 00
1.6416E-03  1.0430E-04  3.8338E-04  5.1132E-01  1.8334E-02  1.2020E-06  2.3507E-06  1.0820E 00  1.0823E 00
1.7328E-03  1.0400E-04  4.2870E-04  5.1056E-01  5.6895E-02  3.8163E-07  7.4748E-07  1.0724E 00  1.0730E 00
1.8240E-03  8.7219E-05  4.7376E-04  5.0974E-01  8.0729E-02  2.7499E-07  5.3948E-07  1.0539E 00  1.0551E 00
1.9152E-03  6.8427E-05  5.1826E-04  5.0870E-01  1.1700E-01  2.0127E-07  3.9566E-07  1.0246E 00  1.0252E 00
2.0064E-03  6.8966E-05  5.6242E-04  5.0759E-01  1.3853E-01  1.5184E-07  3.7795E-07  9.8676E-01  9.8755E-01
2.0976E-03  6.4818E-05  6.0624E-04  5.0641E-01  1.9733E-01  1.5090E-07  2.9798E-07  9.3167E-01  9.3238E-01
2.1888E-03  6.1321E-05  6.4969E-04  5.0516E-01  4.3524E-01  7.2529E-08  1.4556E-07  8.3090E-01  8.3211E-01
2.2800E-03  1.5718E-04  6.9421E-04  5.0448E-01  7.4979E-01  3.9842E-08  7.8976E-08  5.0000E-01  5.0015E-01
2.3712E-03  2.7164E-04  7.3928E-04  5.0408E-01 -6.5490E-02  1.5898E-07  3.1538E-07  2.4514E-01  2.4497E-01
2.4624E-03  8.3218E-05  7.8361E-04  5.0341E-01 -4.8942E-02  2.6403E-07  5.2448E-07  1.5916E-01  1.5994E-01
2.5536E-03  2.7974E-05  8.2499E-04  5.0164E-01 -3.7478E-01  3.4666E-07  6.9106E-07  9.1623E-02  9.1873E-02
2.6448E-03  3.6619E-05  8.6345E-04  4.9888E-01 -1.7507E-01  8.2417E-07  1.6520E-06  5.6403E-02  5.6365E-02
2.7360E-03  5.0262E-05  9.0391E-04  4.9704E-01 -2.5756E-01  8.3234E-07  1.6746E-06  4.2800E-02  4.2561E-02
2.8272E-03  8.0366E-05  9.4569E-04  4.9579E-01 -1.5462E-01  1.7068E-06  3.4427E-06  2.7155E-02  2.6817E-02
2.9184E-03  2.0124E-04  9.8893E-04  4.9511E-01  1.8301E-02 -1.4579E-05 -2.9446E-05  2.4407E-02  2.4915E-02
3.0096E-03  4.8096E-05  1.0329E-03  4.9472E-01 -2.2788E-02  1.3252E-05  2.6788E-05  2.2843E-02  2.3368E-02
3.1008E-03  2.2471E-05  1.0685E-03  4.9164E-01 -2.3789E-02  1.3300E-05  2.7053E-05  2.1659E-02  2.2133E-02
3.1920E-03  1.8568E-05  1.1013E-03  4.8786E-01 -9.8798E-03  3.3812E-05  6.9307E-05  2.1029E-02  2.1496E-02
3.2832E-03  2.2745E-05  1.1343E-03  4.8438E-01 -2.8346E-02  1.2018E-05  2.4812E-05  2.0168E-02  2.0679E-02
3.3744E-03  2.2269E-05  1.1670E-03  4.8096E-01 -2.8824E-02  1.2267E-05  2.5505E-05  1.9256E-02  1.9736E-02
3.4656E-03  1.6588E-05  1.1964E-03  4.7681E-01 -2.9134E-02  7.2003E-06  1.5101E-05  1.7908E-02  1.8541E-02
3.5568E-03  1.5090E-05  1.2234E-03  4.7216E-01 -5.7799E-02  5.0934E-06  1.0787E-05  1.6033E-02  1.6619E-02
3.6480E-03  1.4515E-05  1.2485E-03  4.6724E-01 -8.8055E-02  4.5098E-06  9.6520E-06  1.3891E-02  1.4363E-02
3.7392E-03  1.0071E-05  1.2671E-03  4.6083E-01 -1.1673E-01  4.0498E-06  8.7881E-06  1.1626E-02  1.2086E-02
3.8304E-03  7.6930E-06  1.2775E-03  4.5256E-01 -1.4266E-01  3.5814E-06  7.9137E-06  9.3274E-03  9.6287E-03
3.9216E-03  1.0103E-05  1.2900E-03  4.4522E-01 -1.2536E-01  4.3419E-06  9.7521E-06  7.4479E-03  7.7569E-03
4.0128E-03  4.6915E-06  1.2824E-03  4.3322E-01 -1.3366E-01  3.9246E-06  9.0592E-06  5.7757E-03  6.0629E-03
4.1040E-03  4.3467E-06  1.2648E-03  4.1930E-01 -1.3282E-01  3.7093E-06  8.8464E-06  4.3111E-03  4.5659E-03
4.1952E-03  3.0060E-06  1.2266E-03  4.0107E-01 -1.2226E-01  3.5296E-06  8.8004E-06  3.0539E-03  3.2748E-03
4.2864E-03  1.8404E-06  1.1500E-03  3.7467E-01 -1.6528E-01  2.8960E-06  7.7295E-06  2.0042E-03  2.1874E-03
4.3776E-03  1.2609E-06  1.0316E-03  3.3983E-01 -9.2100E-02  2.3445E-06  6.8989E-06  1.1620E-03  1.2981E-03
4.4688E-03  6.1646E-07  8.2472E-04  2.8659E-01 -1.0394E-01  1.7385E-06  6.0662E-06  5.2726E-04  6.0517E-04
4.5600E-03  1.1948E-11  5.5879E-08  1.0001E-01 -9.2024E-02  1.4750E-07  1.4748E-06  1.0021E-04 -8.0070E-07
```

TABLE 5.7b. Computer output for simulation of concentration of K^+ in solution using calculated D_s values for Brookston clay.

```
DS FOR POTASSIUM AND SIMULATION OF CONCENTRATION (BROOKSTON CLAY)        RKS        INTEGRATION

 LAMBDA        D           E            THLA        LATHAD       THDS        DS          SEFLA       SEF1
0.0         6.5184E-05 -2.1840E-04   5.3000E-01   3.2592E-04  3.0852E-05  5.8212E-05  9.6503E-01  9.6500E-01
3.6400E-05  6.5258E-06 -1.9917E-04   5.2818E-01   3.1668E-04  3.0743E-05  5.8206E-05  9.6496E-01  9.6497E-01
7.2800E-05  6.5176E-06 -1.8008E-04   5.2636E-01   3.0470E-04  3.0874E-05  5.8656E-05  9.6493E-01  9.6493E-01
1.0920E-04  6.9936E-06 -1.6111E-04   5.2462E-01   2.9972E-04  3.0293E-05  5.7743E-05  9.6489E-01  9.6489E-01
1.4560E-04  1.0248E-05 -1.4221E-04   5.2327E-01   2.8330E-04  3.0895E-05  5.9042E-05  9.6485E-01  9.6486E-01
1.8200E-04  1.1627E-05 -1.2337E-04   5.2214E-01   2.7182E-04  3.1026E-05  5.9421E-05  9.6482E-01  9.6482E-01
2.1840E-04  1.4841E-05 -1.0456E-04   5.2123E-01   2.6132E-04  3.1036E-05  5.9543E-05  9.6478E-01  9.6479E-01
2.5480E-04  2.0515E-05 -8.5765E-05   5.2055E-01   2.5666E-04  3.0232E-05  5.8269E-05  9.6475E-01  9.6475E-01
2.9120E-04  3.3211E-05 -6.6953E-05   5.2008E-01   2.3970E-04  3.1176E-05  5.9945E-05  9.6471E-01  9.6471E-01
3.2760E-04  1.2835E-05 -4.8274E-05   5.1931E-01   7.9456E-03  9.0336E-07  1.7395E-06  9.6386E-01  9.6414E-01
3.6400E-04  1.2070E-05 -2.9703E-05   5.1840E-01   1.2350E-02  5.6181E-07  1.0837E-06  9.6222E-01  9.6244E-01
4.0040E-04  1.3001E-05 -1.1197E-05   5.1749E-01   1.4683E-02  4.5729E-07  8.8367E-07  9.5998E-01  9.6018E-01
4.3680E-04  1.2987E-05  7.2420E-06   5.1658E-01   8.5614E-03  7.5404E-07  1.4597E-06  9.5819E-01  9.5848E-01
4.7320E-04  1.2977E-05  2.5615E-05   5.1567E-01   9.6156E-03  6.4353E-07  1.2479E-06  9.5637E-01  9.5667E-01
5.0960E-04  1.2970E-05  4.3921E-05   5.1476E-01   1.3062E-02  4.5301E-07  8.8005E-07  9.5399E-01  9.5472E-01
5.4600E-04  1.2958E-05  6.2162E-05   5.1385E-01   2.6913E-02  2.1267E-07  4.1387E-07  9.4934E-01  9.4988E-01
5.8240E-04  1.2954E-05  8.0336E-05   5.1294E-01   2.9034E-02  1.9091E-07  3.7218E-07  9.4337E-01  9.4385E-01
6.1880E-04  1.2939E-05  9.8444E-05   5.1203E-01   3.6111E-02  1.4878E-07  2.9057E-07  9.3550E-01  9.3628E-01
6.5520E-04  1.2925E-05  1.1649E-04   5.1112E-01   4.3682E-02  1.1978E-07  2.3435E-07  9.2529E-01  9.2597E-01
6.9160E-04  1.2921E-05  1.3446E-04   5.1021E-01   4.7192E-02  1.0793E-07  2.1153E-07  9.1310E-01  9.1373E-01
7.2800E-04  7.3725E-06  1.5208E-04   5.0890E-01   7.0092E-02  7.4939E-08  1.4726E-07  8.9622E-01  8.9715E-01
7.6440E-04  7.0656E-06  1.6940E-04   5.0733E-01   8.0731E-02  6.8370E-08  1.3477E-07  8.7480E-01  8.7562E-01
8.0080E-04  6.4103E-06  1.8647E-04   5.0558E-01   8.3878E-02  6.2058E-06  1.2275E-07  8.4931E-01  8.5015E-01
8.3720E-04  5.8598E-06  2.0328E-04   5.0368E-01   1.0576E-01  4.7544E-08  9.4394E-08  8.1407E-01  8.1471E-01
6.7360E-04  5.3999E-06  2.1980E-04   5.0161E-01   1.7042E-01  2.8172E-08  5.6163E-08  7.5903E-01  7.6124E-01
9.1000E-04  6.8261E-06  2.3614E-04   4.9950E-01   2.5060E-01  1.9284E-08  3.8606E-08  6.7000E-01  6.7243E-01
9.4640E-04  6.3548E-06  2.5260E-04   4.9768E-01   3.7758E-01  8.6222E-09  1.7325E-08  5.0226E-01  5.0482E-01
9.8280E-04  6.3373E-06  2.6893E-04   4.9586E-01  -7.2494E-02  1.3319E-08  2.6860E-08  2.2320E-01  2.2549E-01
1.0192E-03  6.3033E-06  2.8512E-04   4.9404E-01  -3.7251E-01  3.2753E-08  6.6297E-08  1.0678E-01  1.0841E-01
1.0556E-03  6.2923E-06  3.0119E-04   4.9222E-01  -3.5469E-01  6.0291E-08  1.2249E-07  5.9401E-02  6.1242E-02
1.0920E-03  6.2802E-06  3.1712E-04   4.9040E-01  -2.7248E-01  1.0539E-07  2.1492E-07  3.4000E-02  3.5219E-02
1.1284E-03  3.5013E-06  3.3188E-04   4.8767E-01  -2.7101E-01  1.1487E-07  2.3555E-07  2.0548E-02  2.0928E-02
1.1648E-03  2.8926E-06  3.4547E-04   4.8409E-01  -3.0875E-01  1.5391E-07  3.1795E-07  1.1119E-02  1.1365E-02
1.2012E-03  2.5305E-06  3.5805E-04   4.7990E-01  -1.7446E-01  3.5210E-07  7.3270E-07  5.9554E-03  5.9954E-03
1.2376E-03  4.1586E-06  3.7195E-04   4.7702E-01  -1.1494E-02  4.5783E-06  1.0436E-05  5.6240E-03  6.0491E-03
1.2740E-03  4.8558E-06  3.8615E-04   4.7453E-01  -2.4185E-02  2.4241E-06  5.1084E-06  5.2600E-03  5.6752E-03
1.3104E-03  4.5407E-06  4.0024E-04   4.7210E-01  -2.3221E-02  2.3344E-06  4.9448E-06  4.8960E-03  5.3062E-03
1.3468E-03  2.8125E-06  4.1284E-04   4.6869E-01  -2.0865E-02  2.2597E-06  4.8212E-06  4.5320E-03  4.9369E-03
1.3832E-03  2.7121E-06  4.2463E-04   4.6489E-01  -2.6435E-02  2.1700E-06  4.6678E-06  4.1680E-03  4.5675E-03
1.4196E-03  2.0331E-06  4.3476E-04   4.6010E-01  -2.9736E-02  2.0677E-06  4.4941E-06  3.8040E-03  4.1979E-03
1.4560E-03  1.5317E-06  4.4249E-04   4.5591E-01  -3.3162E-02  1.9533E-06  4.3034E-06  3.4400E-03  3.8275E-03
1.4924E-03  1.3326E-06  4.4818E-04   4.4665E-01  -3.6717E-02  1.8262E-06  4.0886E-06  3.0760E-03  3.4576E-03
1.5288E-03  1.3819E-06  4.5323E-04   4.3932E-01  -4.0400E-02  1.6859E-06  3.8375E-06  2.7120E-03  3.0866E-03
1.5652E-03  1.1212E-06  4.5615E-04   4.3097E-01  -4.4213E-02  1.5319E-06  3.5546E-06  2.3480E-03  2.7154E-03
1.6016E-03  7.3224E-07  4.5337E-04   4.1944E-01  -4.7740E-02  1.3640E-06  3.2519E-06  1.9840E-03  2.3431E-03
1.6380E-03  5.9260E-07  4.4541E-04   4.0526E-01  -4.6490E-02  1.2029E-06  2.9683E-06  1.6200E-03  1.9698E-03
1.6744E-03  4.1317E-07  4.2894E-04   3.8661E-01  -5.9640E-02  1.0035E-06  2.5957E-06  1.2560E-03  1.5951E-03
1.7108E-03  2.7787E-07  4.0014E-04   3.6155E-01  -6.3448E-02  8.0266E-07  2.2201E-06  9.0107E-04  1.2198E-03
1.7472E-03  1.7920E-07  3.5454E-04   3.2792E-01  -6.6622E-02  6.5648E-07  2.0029E-06  5.8064E-04  8.8644E-04
1.7836E-03  7.6241E-08  2.6814E-04   2.7279E-01  -7.7678E-02  3.5731E-07  1.3099E-06  2.8029E-04  5.6281E-04
1.8200E-03  6.2742E-13  8.8185E-09   1.2000E-01   2.9285E-02  3.5542E-08  2.9617E-07  5.1850E-09  3.9031E-07


DSEF,SSLOPE,DRVEL=   -0.138661E-03    0.448335E 05    0.170535E-11
```

FIGURE 5.19.

(a) Reduced moisture content $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ as a function of λ and reduced concentration $C_2 = (C-C_n)/(C_o-C_n)$ as a function of λ.

(b) Reduced water content Θ as a function of χ_w and reduced concentration C_2 as a function of χ_s.

(c) Reduced water content Θ and reduced concentration C_2 as functions of ψ_w and ψ_s, respectively.

(d) Reduced water content Θ and reduced concentration C_2 as functions of ω_w and ω_s, respectively.

(Akuse clay)

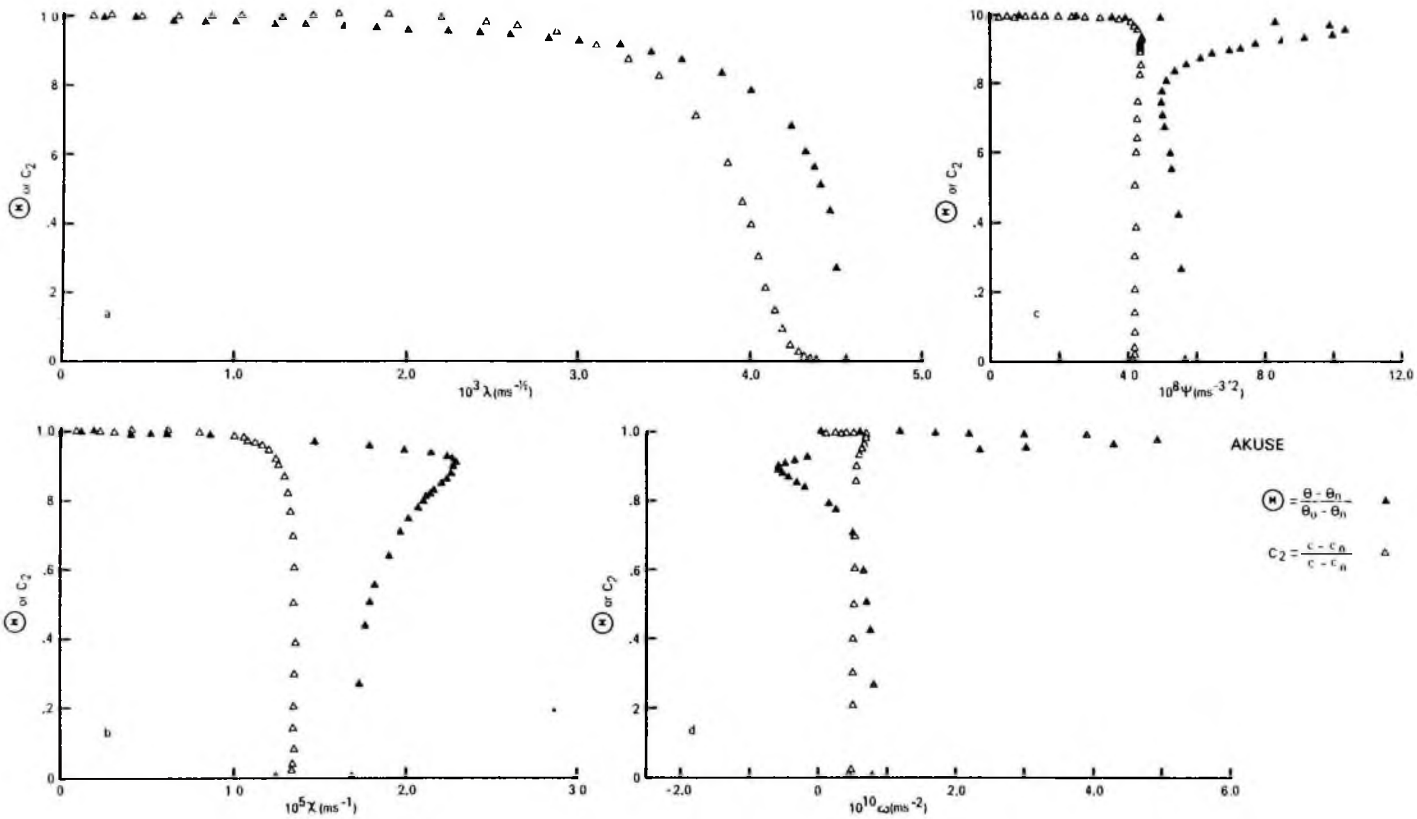
1.0
.8
.6
.4
.2
0
Θ or C2
a
0
1.0
2.0
3.0
4.0
5.0
$10^3 \lambda$ (ms$^{-1/2}$)
c
0
4.0
8.0
12.0
$10^8 \Psi$ (ms$^{-3/2}$)
b
0
1.0
2.0
3.0
$10^5 \chi$ (ms^{-1})
d
-2.0
0
2.0
4.0
6.0
$10^{10} \omega$ (ms^{-2})
AKUSE
$\Theta = \frac{\theta - \theta_n}{\theta_0 - \theta_n}$ ▲
$C_2 = \frac{c - c_n}{c - c_n}$ △

Figure 5.19

LATHAD, θD_s (THDS), D_s, interpolated experimental concentration of K^+ (SEELA) and simulated concentration of K^+ (SEE1). The interpolated experimental data obtained with the NLFGEN (non linear function generator) algorithm of CSMP which interpolates between data points using Lagrange quadratic interpolation is plotted in figures 5.18a and 5.18b for comparison. It is observed from Tables 5.7a, 5.7b and figures 5.18a and 5.18b that simulated and experimental values of $c(\lambda)$ for K^+ agree very well.

Finally, we conclude that given $D_s(\lambda)$ or $D_s(\theta)$ and $D(\lambda)$ or $D(\theta)$, the computer programs described in Chapter 4 simulated $\theta(\lambda)$, $c(\lambda)$ for both Cl^- and K^+ which agree very well with experimentally determined data. Also excellent agreement is obtained between simulated $c(\lambda)$ for Cl^- and $c(\lambda)$ calculated using a computer program for the analytical solution.

5.6 Simulated Water Content Profile and Salt Content Profiles for Vertical Infiltration

The simulated water content profile with depth and chloride content profile with depth for various time periods was based on the first four terms of the expansion

$$z(\theta) = \lambda(\theta)t^{1/2} + \chi_w(\theta)t + \psi_w(\theta)t^{3/2} + \omega_w(\theta)t^2; \text{ and}$$

$$z(c) = \lambda(c)t^{1/2} + \chi_s(c)t + \psi_s(c)t^{3/2} + \omega_s(c)t^2 .$$

Figures 5.19a, 5.19b, 5.19c and 5.19d present the $\Theta(\lambda)$, $C_2(\lambda)$,

$\Theta(\chi_w)$, $C_2(\chi_s)$, $\Theta(\psi_w)$, $\Theta(\psi_w)$ and $C_2(\omega_s)$ data for Akuse clay. In these plots, Θ is the reduced water content θ, defined as $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ and the reduced concentration C_2 is defined similarly as $C_2 = (c-c_n)/(c_o-c_n)$. Similar graphical representations for Brookston clay are presented in figures 5.20a, 5.20b, 5.20c and 5.20d. The $\Theta(\lambda)$ and $C_2(\lambda)$ plots are the smoothed experimental data interpolated with the CSMP algorithm NLFGEN which provides a Lagrange quadratic interpolation between experimental data points given in a FUNCTION card. As mentioned earlier, the wetting front is abrupt and sharp whilst the 'salt front' which lags behind the wetting front is dispersed.

The χ_w, χ_s, ψ_w, ψ_s, ω_w and ω_s data (Tables 5.8a and 5.8b) were obtained with the computer program described in Chapter 4 and the experimental data inputs $\theta(\lambda)$, $c(\lambda)$ and hydraulic conductivity as a function of water content $K(\theta)$ (figures 5.5a, 5.5b, 5.6a, 5.6b, 5.14a and 5.14b). Figures 5.19b and 5.20b indicate that for Θ or C_2, the χ_w values are greater than χ_s with the former attaining a maximum near saturation (for example, maximum χ_w for Akuse clay is at $\Theta = 0.9$) whilst χ_s attains a maximum at low chloride concentrations corresponding with the drier region in the soil column (e.g. for Akuse clay maximum χ_s is at C_2=0.02). Similar trends are observed with $\Theta(\psi_w)$ and $C_2(\psi_s)$; $\Theta(\omega_w)$ and $C_2(\omega_w)$ relationships. In all cases, the maximum for ψ_w and ω_w for water occurs near higher water contents whilst the maximum for ψ_s or ω_s for salt occurs at lower salt contents corresponding to low water contents.

Table 5.9a and 5.9b show how well the boundary conditions listed in Tables 4.3 were met for Akuse clay and Brookston clay, respectively. Definitions for RVEL, QVEL, SVEL, RVELS, QVELS and SVELS in Table 5.9a and 5.9b are as already given in the text (see equations 4.130 to 4.135). In Tables 5.9a and 5.9b the soil water diffusivity D and dispersion coefficient DS are also printed. Note that the FINTIM values for RVEL, QVEL, SVEL, RVELS, QVELS and SVELS, even though not zero, are very small indeed. For example, RVEL values in Table 5.9a are generally of the order of magnitude 10^{-5} to 10^{-7} but that at $\lambda = 4.56 \times 10^{-3}$ $ms^{-1/2}$ is 10^{-13}.

It is pertinent at this stage to compare the magnitudes of λ, χ, ψ and ω for water and salt (see Tables 5.8a and 5.8b). It is observed that for Akuse clay λ is of the order of magnitude 10^{-3}, the order of magnitude of χ is 10^{-5} whilst ψ and ω are of the magnitude 10^{-8} and 10^{-10}, respectively. Similarly, the order of magnitude of λ, χ, ψ and ω for Brookston clay are 10^{-3}, 10^{-6}, 10^{-8} and 10^{-11}, respectively. This is an indication that, as expected, the dominant terms in the series expansion are λ and χ. As to whether the expansion may be truncated to the first two terms to obtain a good approximation depends on the magnitudes of the terms $\lambda t^{1/2}$, χt, $\psi t^{3/2}$ and ωt^2 calculated with the computer program in figures 4.10 and 4.11. Representative data showing the percent contribution of $\lambda t^{1/2}$, χt, $\psi t^{3/2}$ and ωt^2 to the depth of vertical infiltration and the vertical distance moved by chloride are presented in Tables 5.10a, 5.10b, 5.11a and 5.11b. The percent contribution of each of the terms in these tables was obtained by dividing $\lambda t^{1/2}$, χt, $\psi t^{3/2}$, or ωt^2 value for a particular value of $\Theta = (\theta-\theta_n)/\theta_o-\theta_n)$ or $C_2 = (c-c_n)/(c_o-c_n)$ by the depth z corresponding to that Θ or C_2 and multiplying by 100. Data in Tables 5.10a, 5.10b, 5.11a and 5.11b indicate that at the onset of and during the initial

FIGURE 5.20.

(a) Reduced water content $\Theta = (\theta-\theta_n)/(\theta_o-\theta_n)$ and reduced concentration $C_2 = (C-C_n)/(C_o-C_n)$ plotted as functions of λ.

(b) Reduced water content Θ and reduced concentration C_2 plotted as functions of χ_w and χ_s, respectively.

(c) Reduced water content Θ and reduced concentration C_2 as functions of ψ_w and ψ_s, respectively.

(d) Reduced water content Θ and reduced concentration C_2 plotted against ω_w and ω_s, respectively.

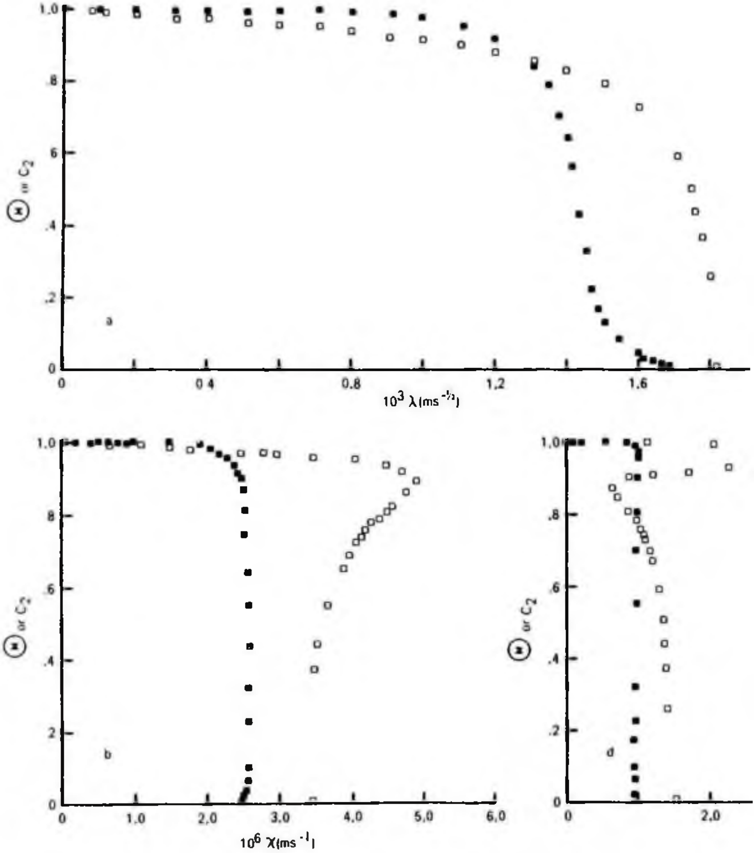
1.0
.8
.6
.4
.2
0
Ⓧ or C_2
a
0
0.4
0.8
1.2
1.6
$10^3\ \lambda\ (ms^{-1/2})$
1.0
.8
.6
.4
.2
0
Ⓧ or C_2
b
0
1.0
2.0
3.0
4.0
5.0
6.0
$10^6\ \chi\ (ms^{-1})$
1.0
.8
.6
.4
.2
0
Ⓧ or C_2
d
0
2.0

Figure 5.20

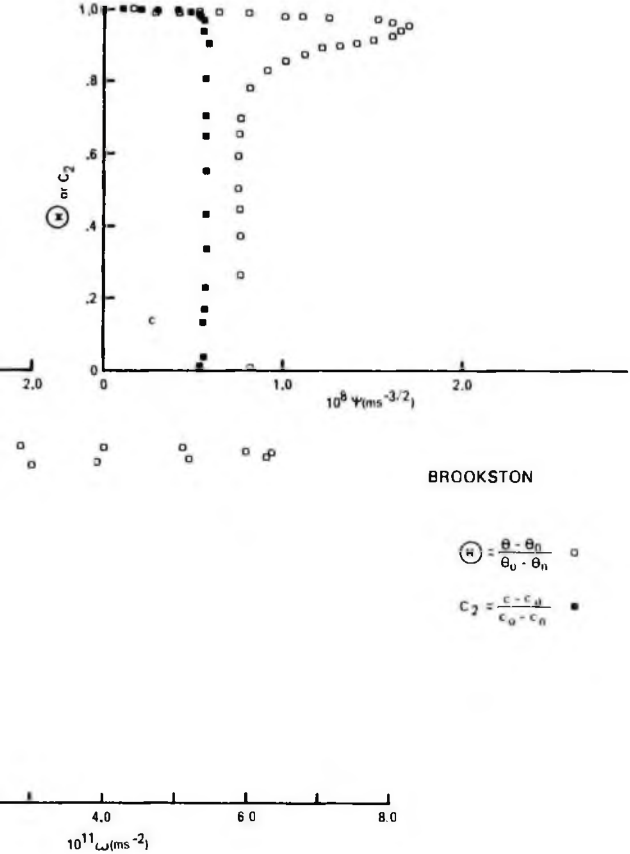
1.0
.8
.6
.4
.2
0
⊖ or C_2
2.0
0
1.0
2.0
$10^8\,\Psi(\mathrm{ms}^{-3/2})$
4.0
6.0
8.0
$10^{11}\,\omega(\mathrm{ms}^{-2})$
BROOKSTON
$\ominus = \frac{\theta - \theta_n}{\theta_0 - \theta_n}$ ○
$C_2 = \frac{c - c_n}{c_0 - c_n}$ ●

TABLE 5.8a. Computer output for χ_w, χ_s, ψ_w, ψ_s, ω_w and ω_s for Akuse clay.

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CHI,PSI, AND OMEGA FOR WATER AND SALT FLOW (AKUSE CLAY)                    SINF      INTEGRATION

  LAMDA        CTHETA       CHI          PSI          OMEGA        CSEE         CHIS         PSIS         CMEGAS
 0.0          1.0000E 00   0.0          0.0          0.0          1.0000E 00   0.0          0.0          0.0
 9.1200E-05   9.9786E-01   1.2434E-06   1.3142E-08   1.2078E-10   9.9990E-01   4.1751E-07   1.7162E-09   3.8363E-12
 1.8240E-04   9.9572E-01   2.4391E-06   2.5010E-08   2.2010E-10   9.9980E-01   8.3371E-07   3.4166E-09   7.5590E-12
 2.7360E-04   9.9358E-01   3.5881E-06   3.5680E-08   3.0031E-10   9.9970E-01   1.2486E-06   5.1017E-09   1.1172E-11
 3.6480E-04   9.9144E-01   4.6914E-06   4.5228E-08   3.6356E-10   9.9960E-01   1.6623E-06   6.7719E-09   1.4680E-11
 4.5600E-04   9.8930E-01   5.7501E-06   5.3722E-08   4.1189E-10   9.9950E-01   2.0747E-06   8.4275E-09   1.8087E-11
 5.4720E-04   9.8715E-01   6.7651E-06   6.1228E-08   4.4709E-10   9.9941E-01   2.4860E-06   1.0069E-08   2.1400E-11
 6.3840E-04   9.8516E-01   7.7382E-06   6.7824E-08   4.7101E-10   9.9931E-01   2.8961E-06   1.1698E-08   2.4624E-11
 7.2960E-04   9.8338E-01   8.6752E-06   7.3672E-08   4.8633E-10   9.9921E-01   3.3051E-06   1.3314E-08   2.7757E-11
 8.2080E-04   9.8160E-01   9.5782E-06   7.8839E-08   4.9431E-10   9.9911E-01   3.7130E-06   1.4917E-08   3.0806E-11
 9.1200E-04   9.7981E-01   1.0448E-05   8.3365E-08   4.9583E-10   9.9901E-01   4.1199E-06   1.6509E-08   3.3776E-11
 1.0032E-03   9.7803E-01   1.1288E-05   8.7338E-08   4.9216E-10   9.9891E-01   4.5258E-06   1.8090E-08   3.6668E-11
 1.0944E-03   9.7624E-01   1.2100E-05   9.0818E-08   4.8418E-10   9.9881E-01   4.9307E-06   1.9659E-08   3.9487E-11
 1.1856E-03   9.7446E-01   1.2885E-05   9.3829E-08   4.7239E-10   9.9871E-01   5.3348E-06   2.1218E-08   4.2239E-11
 1.2768E-03   9.7268E-01   1.3643E-05   9.6394E-08   4.5727E-10   9.9861E-01   5.7379E-06   2.2767E-08   4.4923E-11
 1.3680E-03   9.7089E-01   1.4374E-05   9.8535E-08   4.3923E-10   9.9851E-01   6.1402E-06   2.4306E-08   4.7536E-11
 1.4592E-03   9.6911E-01   1.5079E-05   1.0027E-07   4.1867E-10   9.9841E-01   6.5417E-06   2.5836E-08   5.0094E-11
 1.5504E-03   9.6732E-01   1.5759E-05   1.0163E-07   3.9592E-10   9.9831E-01   6.9424E-06   2.7358E-08   5.2596E-11
 1.6416E-03   9.6554E-01   1.6413E-05   1.0263E-07   3.7136E-10   9.9822E-01   7.3424E-06   2.8872E-08   5.5053E-11
 1.7328E-03   9.6376E-01   1.7042E-05   1.0328E-07   3.4530E-10   9.9812E-01   7.7418E-06   3.0379E-08   5.7465E-11
 1.8240E-03   9.6174E-01   1.7646E-05   1.0362E-07   3.1797E-10   9.9802E-01   8.1404E-06   3.1879E-08   5.9835E-11
 1.9152E-03   9.5906E-01   1.8217E-05   1.0354E-07   2.8944E-10   9.9792E-01   8.5385E-06   3.3372E-08   6.2166E-11
 2.0064E-03   9.5638E-01   1.8753E-05   1.0304E-07   2.6007E-10   9.9782E-01   8.9359E-06   3.4859E-08   6.4464E-11
 2.0976E-03   9.5371E-01   1.9254E-05   1.0217E-07   2.3031E-10   9.9772E-01   9.3329E-06   3.6340E-08   6.6729E-11
 2.1888E-03   9.5103E-01   1.9722E-05   1.0095E-07   2.0056E-10   9.9009E-01   9.7118E-06   3.7648E-08   6.8104E-11
 2.2800E-03   9.4977E-01   2.0164E-05   9.9481E-08   1.7105E-10   9.8696E-01   1.0065E-05   3.8716E-08   6.8334E-11
 2.3712E-03   9.4869E-01   2.0593E-05   9.7893E-08   1.4173E-10   9.8448E-01   1.0408E-05   3.9696E-08   6.8201E-11
 2.4624E-03   9.4689E-01   2.1005E-05   9.6164E-08   1.1274E-10   9.8200E-01   1.0743E-05   4.0602E-08   6.7782E-11
 2.5536E-03   9.4223E-01   2.1385E-05   9.4160E-08   8.4637E-11   9.7952E-01   1.1069E-05   4.1441E-08   6.7134E-11
 2.6448E-03   9.3765E-01   2.1700E-05   9.1690E-08   5.8954E-11   9.7339E-01   1.1386E-05   4.2207E-08   6.6264E-11
 2.7360E-03   9.3498E-01   2.1981E-05   8.9000E-08   3.4954E-11   9.6348E-01   1.1679E-05   4.2810E-08   6.4985E-11
 2.8272E-03   9.3230E-01   2.2233E-05   8.6154E-08   1.2503E-11   9.5356E-01   1.1951E-05   4.3268E-08   6.3446E-11
 2.9184E-03   9.2962E-01   2.2457E-05   8.3170E-08  -8.3207E-12   9.4365E-01   1.2202E-05   4.3612E-08   6.1784E-11
 3.0096E-03   9.2638E-01   2.2654E-05   8.0068E-08  -2.7435E-11   9.3269E-01   1.2438E-05   4.3865E-08   6.0086E-11
 3.1008E-03   9.1836E-01   2.2794E-05   7.6777E-08  -4.2738E-11   9.1286E-01   1.2650E-05   4.4010E-08   5.8430E-11
 3.1920E-03   9.1033E-01   2.2861E-05   7.3339E-08  -5.2791E-11   8.9304E-01   1.2838E-05   4.4056E-08   5.6903E-11
 3.2832E-03   9.0230E-01   2.2863E-05   6.9867E-08  -5.7919E-11   8.7321E-01   1.3006E-05   4.4030E-08   5.5537E-11
 3.3744E-03   8.9427E-01   2.2806E-05   6.6445E-08  -5.8661E-11   8.4529E-01   1.3155E-05   4.3948E-08   5.4361E-11
 3.4656E-03   8.8432E-01   2.2692E-05   6.3142E-08  -5.5426E-11   8.1199E-01   1.3281E-05   4.3814E-08   5.3425E-11
 3.5568E-03   8.7361E-01   2.2516E-05   6.0049E-08  -4.8121E-11   7.7420E-01   1.3387E-05   4.3642E-08   5.2734E-11
 3.6480E-03   8.6178E-01   2.2284E-05   5.7219E-08  -3.7608E-11   7.2933E-01   1.3474E-05   4.3442E-08   5.2271E-11
 3.7392E-03   8.4618E-01   2.1991E-05   5.4750E-08  -2.4253E-11   6.7550E-01   1.3542E-05   4.3223E-08   5.2021E-11
 3.8304E-03   8.2798E-01   2.1628E-05   5.2800E-08  -8.5862E-12   6.0776E-01   1.3591E-05   4.2992E-08   5.1949E-11
 3.9216E-03   8.0939E-01   2.1210E-05   5.1314E-08   7.9673E-12   5.1527E-01   1.3620E-05   4.2755E-08   5.2019E-11
 4.0128E-03   7.8188E-01   2.0731E-05   5.0436E-08   2.4400E-11   3.3796E-01   1.3626E-05   4.2514E-08   5.2220E-11
 4.1040E-03   7.4930E-01   2.0192E-05   5.0229E-08   3.9527E-11   2.1082E-01   1.3603E-05   4.2278E-08   5.2632E-11
 4.1952E-03   7.0648E-01   1.9598E-05   5.0710E-08   5.2286E-11   8.5374E-02   1.3545E-05   4.2053E-08   5.3307E-11
 4.2864E-03   6.4338E-01   1.8956E-05   5.1831E-08   6.1974E-11   1.9936E-02   1.3443E-05   4.1867E-08   5.4887E-11
 4.3776E-03   5.6094E-01   1.8281E-05   5.3403E-08   6.9091E-11   6.7177E-03   1.3294E-05   4.1898E-08   6.0145E-11
 4.4688E-03   4.3451E-01   1.7594E-05   5.5173E-08   7.5005E-11   5.8699E-04   1.3079E-05   4.4708E-08   1.0113E-10
 4.5600E-03   0.0          1.6906E-05   5.6914E-08   7.4399E-11   0.0          1.2584E-05   1.0839E-06   1.5456E-08
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TABLE 5.8b. Computer output of χ_w, χ_s, ψ_w, ψ_s, ω_w and ω_s for Brookston clay.

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CHI.PSI. AND OMEGA FOR WATER AND SALT FLOW (BROOKSTON CLAY)              SIMP     INTEGRATION

 LAMDA        CTHETA       CHI          PSI          OMEGA        CSEE         CHIS         PSIS         OMEGAS
C.0          1.0000E 00   0.0          C.0          0.0          1.0000E 00   0.0          0.0          0.0
3.6400E-05   9.9556E-01   3.5107E-07   2.8493E-09   2.0641E-11   9.9996E-01   8.0666E-08   2.0948E-10   4.2722E-13
7.2800E-05   9.9112E-01   6.7472E-07   5.1827E-09   3.4986E-11   9.9992E-01   1.6122E-07   4.1822E-10   8.5127E-13
1.0920E-04   9.8724E-01   9.7221E-07   7.0653E-09   4.4379E-11   9.9989E-01   2.4168E-07   6.2622E-10   1.2722E-12
1.4560E-04   9.8502E-01   1.2546E-06   8.6903E-09   5.1089E-11   9.9985E-01   3.2202E-07   8.3352E-10   1.6900E-12
1.8200E-04   9.8280E-01   1.5245E-06   1.0129E-08   5.6191E-11   9.9981E-01   4.0227E-07   1.0401E-09   2.1048E-12
2.1840E-04   9.8059E-01   1.7824E-06   1.1394E-08   5.9793E-11   9.9977E-01   4.8243E-07   1.2461E-09   2.5167E-12
2.5480E-04   9.7837E-01   2.0286E-06   1.2497E-08   6.2097E-11   9.9974E-01   5.6249E-07   1.4514E-09   2.9258E-12
2.9120E-04   9.7615E-01   2.2633E-06   1.3450E-08   6.3286E-11   9.9970E-01   6.4246E-07   1.6562E-09   3.3323E-12
3.2760E-04   9.7393E-01   2.4869E-06   1.4263E-08   6.3524E-11   9.9966E-01   7.2235E-07   1.8604E-09   3.7363E-12
3.6400E-04   9.7171E-01   2.6997E-06   1.4948E-08   6.2956E-11   9.9962E-01   8.0216E-07   2.0640E-09   4.1378E-12
4.0040E-04   9.6949E-01   2.9019E-06   1.5514E-08   6.1713E-11   9.9959E-01   8.8189E-07   2.2671E-09   4.5370E-12
4.3680E-04   9.6727E-01   3.0938E-06   1.5969E-08   5.9911E-11   9.9955E-01   9.6154E-07   2.4697E-09   4.9341E-12
4.7320E-04   9.6505E-01   3.2757E-06   1.6324E-08   5.7652E-11   9.9951E-01   1.0411E-06   2.6718E-09   5.3291E-12
5.0960E-04   9.6283E-01   3.4479E-06   1.6586E-08   5.5029E-11   9.9947E-01   1.1206E-06   2.8735E-09   5.7221E-12
5.4600E-04   9.6061E-01   3.6106E-06   1.6762E-08   5.2119E-11   9.9944E-01   1.2001E-06   3.0748E-09   6.1132E-12
5.8240E-04   9.5839E-01   3.7648E-06   1.6864E-08   4.8999E-11   9.9940E-01   1.2795E-06   3.2756E-09   6.5026E-12
6.1880E-04   9.5617E-01   3.9120E-06   1.6911E-08   4.5763E-11   9.9936E-01   1.3588E-06   3.4761E-09   6.8903E-12
6.5520E-04   9.5395E-01   4.0524E-06   1.6905E-08   4.2437E-11   9.9932E-01   1.4381E-06   3.6761E-09   7.2764E-12
6.9160E-04   9.5173E-01   4.1862E-06   1.6852E-08   3.9050E-11   9.9929E-01   1.5173E-06   3.8759E-09   7.6611E-12
7.2800E-04   9.4780E-01   4.3115E-06   1.6743E-08   3.5636E-11   9.9925E-01   1.5964E-06   4.0753E-09   8.0444E-12
7.6440E-04   9.4337E-01   4.4241E-06   1.6554E-08   3.2217E-11   9.9921E-01   1.6755E-06   4.2744E-09   8.4266E-12
8.0080E-04   9.3893E-01   4.5244E-06   1.6298E-08   2.8876E-11   9.9910E-01   1.7546E-06   4.4732E-09   8.8077E-12
8.3720E-04   9.3449E-01   4.6128E-06   1.5982E-08   2.5670E-11   9.9565E-01   1.8318E-06   4.6616E-09   9.1525E-12
8.7360E-04   9.3005E-01   4.6898E-06   1.5618E-08   2.2643E-11   9.9219E-01   1.9055E-06   4.8299E-09   9.4212E-12
9.1000E-04   9.2561E-01   4.7559E-06   1.5214E-08   1.9827E-11   9.8866E-01   1.9762E-06   4.9815E-09   9.6333E-12
9.4640E-04   9.2117E-01   4.8113E-06   1.4777E-08   1.7241E-11   9.8490E-01   2.0440E-06   5.1181E-09   9.7977E-12
9.8280E-04   9.1673E-01   4.8566E-06   1.4315E-08   1.4904E-11   9.8115E-01   2.1093E-06   5.2416E-09   9.9237E-12
1.0192E-03   9.1229E-01   4.8921E-06   1.3833E-08   1.2817E-11   9.7542E-01   2.1720E-06   5.3530E-09   1.0019E-11
1.0556E-03   9.0785E-01   4.9182E-06   1.3338E-08   1.0982E-11   9.6791E-01   2.2309E-06   5.4472E-09   1.0070E-11
1.0920E-03   9.0341E-01   4.9354E-06   1.2835E-08   9.3944E-12   9.6041E-01   2.2863E-06   5.5267E-09   1.0090E-11
1.1284E-03   8.9551E-01   4.9418E-06   1.2328E-08   8.0994E-12   9.4851E-01   2.3382E-06   5.5923E-09   1.0085E-11
1.1648E-03   8.8663E-01   4.9332E-06   1.1826E-08   7.2185E-12   9.3537E-01   2.3858E-06   5.6423E-09   1.0055E-11
1.2012E-03   8.7784E-01   4.9110E-06   1.1338E-08   6.7037E-12   9.2205E-01   2.4298E-06   5.6805E-09   1.0011E-11
1.2376E-03   8.7163E-01   4.8783E-06   1.0869E-08   6.4630E-12   9.0328E-01   2.4704E-06   5.7086E-09   9.9605E-12
1.2740E-03   8.6541E-01   4.8375E-06   1.0419E-08   6.4125E-12   8.7462E-01   2.5072E-06   5.7267E-09   9.9049E-12
1.3104E-03   8.5844E-01   4.7891E-06   9.9896E-09   6.5282E-12   8.3762E-01   2.5395E-06   5.7340E-09   9.8475E-12
1.3468E-03   8.4956E-01   4.7331E-06   9.5841E-09   6.7933E-12   7.9258E-01   2.5673E-06   5.7322E-09   9.7923E-12
1.3832E-03   8.4068E-01   4.6705E-06   9.2027E-09   7.1763E-12   7.0304E-01   2.5902E-06   5.7224E-09   9.7423E-12
1.4196E-03   8.2798E-01   4.6008E-06   8.8482E-09   7.6680E-12   5.5868E-01   2.6071E-06   5.7039E-09   9.6975E-12
1.4560E-03   8.1200E-01   4.5211E-06   8.5376E-09   8.2777E-12   3.2977E-01   2.6153E-06   5.6750E-09   9.6547E-12
1.4924E-03   7.9602E-01   4.4324E-06   8.2712E-09   8.9081E-12   1.7799E-01   2.6141E-06   5.6405E-09   9.6286E-12
1.5288E-03   7.7863E-01   4.3375E-06   8.0392E-09   9.6099E-12   1.0994E-01   2.6063E-06   5.6057E-09   9.6175E-12
1.5652E-03   7.5717E-01   4.2365E-06   7.8409E-09   1.0429E-11   7.1787E-02   2.5934E-06   5.5686E-09   9.5988E-12
1.6016E-03   7.3015E-01   4.1282E-06   7.6866E-09   1.1150E-11   4.7968E-02   2.5757E-06   5.5262E-09   9.5676E-12
1.6380E-03   6.9463E-01   4.0122E-06   7.5808E-09   1.1855E-11   2.8686E-02   2.5523E-06   5.4763E-09   9.5213E-12
1.6744E-03   6.4722E-01   3.8887E-06   7.5260E-09   1.2408E-11   1.9681E-02   2.5230E-06   5.4186E-09   9.4685E-12
1.7108E-03   5.8605E-01   3.7584E-06   7.5209E-09   1.3032E-11   1.4168E-02   2.4865E-06   5.3502E-09   9.4128E-12
1.7472E-03   5.0615E-01   3.6234E-06   7.5534E-09   1.3485E-11   1.0414E-02   2.4431E-06   5.2720E-09   9.3635E-12
1.7836E-03   3.7049E-01   3.4860E-06   7.6033E-09   1.3087E-11   7.6509E-03   2.3897E-06   5.1804E-09   9.3304E-12
1.8200E-03   1.1194E-05   3.5179E-06   6.3132E-09   1.5693E-11   4.9700E-03   2.0627E-06   2.4363E-09   6.8682E-12
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TABLE 5.9a

Computer output showing how well the boundary conditions listed in Table 4.3 were obtained in the simulation of χ, ψ and ω for both water and salt flow for Akuse clay. Note FINTIM data (i.e. $\lambda = 4.56 \times 10^{-3}$) for RVEL, QVEL, etc.are very small. Explanation for QVEL, RVEL, etc. are as in the text.

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CHI.PSI. AND OMEGA FOR WATER AND SALT FLOW (AKUSE CLAY)                    SIMP     INTEGRATION

  LAMDA         RVEL        QVEL        SVEL        RVELS       QVELS       SVELS       D           DS
0.0         -1.2151E-05  3.6658E-08  6.0441E-11 -3.2982E-07  1.5250E-10  2.4646E-12  8.7417E-05  1.3675E-04
9.1200E-05  -1.1688E-05  3.6648E-08  6.0328E-11 -3.2913E-07  1.5573E-10  2.4695E-12  8.6872E-05  1.2907E-04
1.8240E-04  -1.1235E-05  3.6622E-08  6.0016E-11 -3.2845E-07  1.5883E-10  2.4741E-12  8.7408E-05  1.3752E-04
2.7360E-04  -1.0791E-05  3.6581E-08  5.9540E-11 -3.2779E-07  1.6186E-10  2.4785E-12  8.7398E-05  1.3790E-04
3.6480E-04  -1.0356E-05  3.6525E-08  5.8934E-11 -3.2713E-07  1.6480E-10  2.4825E-12  8.7383E-05  1.3828E-04
4.5600E-04  -9.9312E-06  3.6458E-08  5.8227E-11 -3.2650E-07  1.6764E-10  2.4861E-12  8.7365E-05  1.3866E-04
5.4720E-04  -9.5155E-06  3.6379E-08  5.7445E-11 -3.2588E-07  1.7033E-10  2.4893E-12  8.7342E-05  1.3903E-04
6.3840E-04  -9.1370E-06  3.6298E-08  5.6668E-11 -3.2530E-07  1.7288E-10  2.4922E-12  1.0426E-04  1.3118E-04
7.2960E-04  -8.8048E-06  3.6217E-08  5.5944E-11 -3.2472E-07  1.7535E-10  2.4947E-12  1.0581E-04  1.3971E-04
8.2080E-04  -8.4795E-06  3.6131E-08  5.5203E-11 -3.2416E-07  1.7770E-10  2.4970E-12  1.0419E-04  1.4004E-04
9.1200E-04  -8.1664E-06  3.6039E-08  5.4453E-11 -3.2362E-07  1.7992E-10  2.4989E-12  1.0494E-04  1.4036E-04
1.0032E-03  -7.8961E-06  3.5942E-08  5.3706E-11 -3.2310E-07  1.8202E-10  2.5005E-12  1.0411E-04  1.4068E-04
1.0944E-03  -7.6299E-06  3.5841E-08  5.2968E-11 -3.2260E-07  1.8400E-10  2.5018E-12  1.0406E-04  1.5040E-04
1.1856E-03  -7.3673E-06  3.5736E-08  5.2244E-11 -3.2212E-07  1.8588E-10  2.5027E-12  1.0479E-04  1.4131E-04
1.2768E-03  -7.1083E-06  3.5628E-08  5.1542E-11 -3.2166E-07  1.8762E-10  2.5033E-12  1.0396E-04  1.4162E-04
1.3680E-03  -6.8532E-06  3.5518E-08  5.0864E-11 -3.2123E-07  1.8924E-10  2.5036E-12  1.0313E-04  1.4192E-04
1.4592E-03  -6.6019E-06  3.5405E-08  5.0214E-11 -3.2081E-07  1.9073E-10  2.5036E-12  1.0461E-04  1.4223E-04
1.5504E-03  -6.3543E-06  3.5290E-08  4.9598E-11 -3.2041E-07  1.9213E-10  2.5032E-12  1.0534E-04  1.3414E-04
1.6416E-03  -6.1107E-06  3.5175E-08  4.9018E-11 -3.2003E-07  1.9339E-10  2.5026E-12  1.0369E-04  1.4282E-04
1.7328E-03  -5.8707E-06  3.5058E-08  4.8476E-11 -3.1967E-07  1.9455E-10  2.5017E-12  1.0362E-04  1.3469E-04
1.8240E-03  -5.6042E-06  3.4925E-08  4.7912E-11 -3.1933E-07  1.9560E-10  2.5004E-12  6.9362E-05  1.4343E-04
1.9152E-03  -5.2575E-06  3.4749E-08  4.7222E-11 -3.1901E-07  1.9651E-10  2.4989E-12  6.9277E-05  1.4382E-04
2.0064E-03  -4.9187E-06  3.4573E-08  4.6598E-11 -3.1871E-07  1.9733E-10  2.4971E-12  6.8502E-05  1.3573E-04
2.0976E-03  -4.5879E-06  3.4398E-08  4.6040E-11 -3.1843E-07  1.9803E-10  2.4951E-12  6.8410E-05  1.4460E-04
2.1888E-03  -4.2651E-06  3.4225E-08  4.5550E-11 -2.9882E-07  2.4201E-10  2.3270E-12  6.8313E-05  1.8896E-06
2.2800E-03  -4.1158E-06  3.4145E-08  4.5351E-11 -2.9134E-07  2.5738E-10  2.2565E-12  1.7455E-04  6.0354E-06
2.3712E-03  -3.9904E-06  3.4078E-08  4.5210E-11 -2.8583E-07  2.6762E-10  2.1998E-12  1.7227E-04  6.0905E-06
2.4624E-03  -3.7819E-06  3.3966E-08  4.5017E-11 -2.8071E-07  2.7609E-10  2.1441E-12  8.6040E-05  6.1301E-06
2.5536E-03  -3.2602E-06  3.3684E-08  4.4639E-11 -2.7601E-07  2.8282E-10  2.0893E-12  2.8656E-05  6.1959E-06
2.6448E-03  -2.7698E-06  3.3411E-08  4.4349E-11 -2.6559E-07  2.9431E-10  1.9601E-12  6.8774E-05  1.5857E-06
2.7360E-03  -2.4939E-06  3.3257E-08  4.4243E-11 -2.4999E-07  3.0827E-10  1.7607E-12  6.7968E-05  1.6229E-06
2.8272E-03  -2.2257E-06  3.3108E-08  4.4189E-11 -2.3578E-07  3.1786E-10  1.5766E-12  6.7842E-05  1.6572E-06
2.9184E-03  -1.9652E-06  3.2964E-08  4.4185E-11 -2.2286E-07  3.2408E-10  1.4082E-12  6.8050E-05  1.6854E-06
3.0096E-03  -1.6616E-06  3.2797E-08  4.4238E-11 -2.1003E-07  3.2790E-10  1.2426E-12  2.2629E-05  8.5668E-07
3.1008E-03  -9.5306E-07  3.2395E-08  4.4480E-11 -1.8919E-07  3.2971E-10  9.8064E-13  2.2489E-05  8.7991E-07
3.1920E-03  -3.1194E-07  3.2010E-08  4.4809E-11 -1.7074E-07  3.2683E-10  7.6934E-13  2.2346E-05  8.9928E-07
3.2832E-03   2.6438E-07  3.1643E-08  4.5190E-11 -1.5451E-07  3.2131E-10  5.9566E-13  2.2162E-05  9.1473E-07
3.3744E-03   7.5920E-07  3.1294E-08  4.5590E-11 -1.3452E-07  3.1110E-10  4.0481E-13  2.2084E-05  6.1899E-07
3.4656E-03   1.3079E-06  3.0883E-08  4.6076E-11 -1.1380E-07  2.9784E-10  2.1782E-13  1.6390E-05  5.3599E-07
3.5568E-03   1.8145E-06  3.0462E-08  4.6550E-11 -9.3657E-08  2.8198E-10  6.6136E-14  1.6230E-05  4.6994E-07
3.6480E-03   2.3012E-06  3.0020E-08  4.6982E-11 -7.3453E-08  2.6347E-10 -5.7670E-14  1.3374E-05  3.7309E-07
3.7392E-03   2.8523E-06  2.9463E-08  4.7386E-11 -5.3477E-08  2.4254E-10 -1.5025E-13  8.7852E-06  3.0456E-07
3.8304E-03   3.3352E-06  2.8838E-08  4.7647E-11 -3.4039E-08  2.1758E-10 -1.9069E-13  1.0339E-05  2.0538E-07
3.9216E-03   3.7179E-06  2.8223E-08  4.7639E-11 -1.3831E-08  1.8866E-10 -1.6948E-13  6.0747E-06  1.3175E-07
4.0128E-03   4.1154E-06  2.7331E-08  4.7255E-11  3.7299E-09  1.4699E-10 -1.7002E-13  4.9123E-06  7.1846E-08
4.1040E-03   4.4007E-06  2.6287E-08  4.6362E-11  1.4339E-08  8.8623E-11 -1.3303E-13  3.2971E-06  5.5606E-08
4.1952E-03   4.5502E-06  2.4907E-08  4.4679E-11  1.2292E-08  4.4808E-11 -6.9841E-14  3.3552E-06  4.7781E-08
4.2864E-03   4.4427E-06  2.2843E-08  4.1591E-11  5.2081E-09  1.1784E-11 -9.6933E-14  2.0452E-06  3.9123E-08
4.3776E-03   4.0301E-06  2.0072E-08  3.6966E-11  2.3651E-09  4.8485E-13 -1.3196E-13  1.3443E-06  3.8110E-08
4.4688E-03   3.1617E-06  1.5655E-08  2.9116E-11  3.5556E-10 -8.8735E-12 -1.8097E-13  3.7198E-07  3.6615E-08
4.5600E-03   2.8422E-13 -2.7756E-14 -3.6282E-14  1.3747E-12 -1.2306E-11 -2.1177E-13  0.0         0.0
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TABLE 5.9b

Computer output showing how well the boundary conditions listed in Table 4.3 were obtained in the simulation of χ, ψ and ω for both water and salt flow for Brookston clay. Note FINTIM data (i.e. $\lambda = 1.82 \times 10^{-3}$) for RVEL, QVEL, etc. are very small. Explanation for RVEL, QVEL, etc. are as in the text.

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CHI,PSI, AND OMEGA FOR WATER AND SALT FLOW (BROCKSTON CLAY)        SIMP     INTEGRATION

 LAMDA        RVEL         QVEL         SVEL         RVELS        QVELS        SVELS        D            DS
0.0         -3.2681E-06  5.2000E-09   1.2149E-11  -5.9482E-08  -2.2708E-11  7.7408E-14   6.5153E-05   5.0609E-05
3.6400E-05  -3.0174E-06  5.1960E-09   1.2109E-11  -5.9427E-08  -2.2519E-11  7.7547E-14   6.5195E-06   6.5031E-05
7.2800E-05  -2.7769E-06  5.1849E-09   1.2006E-11  -5.9373E-08  -2.2335E-11  7.7761E-14   6.5272E-06   5.6279E-05
1.0920E-04  -2.5787E-06  5.1708E-09   1.1883E-11  -5.9321E-08  -2.2158E-11  7.7996E-14   2.5937E-05   6.0657E-05
1.4560E-04  -2.4690E-06  5.1602E-09   1.1798E-11  -5.9271E-08  -2.1985E-11  7.8295E-14   1.3062E-05   5.6594E-05
1.8200E-04  -2.3596E-06  5.1474E-09   1.1700E-11  -5.9221E-08  -2.1821E-11  7.8592E-14   1.3056E-05   6.0916E-05
2.1840E-04  -2.2528E-06  5.1327E-09   1.1594E-11  -5.9175E-08  -2.1666E-11  7.8871E-14   1.3053E-05   5.6835E-05
2.5480E-04  -2.1485E-06  5.1164E-09   1.1483E-11  -5.9129E-08  -2.1516E-11  7.9141E-14   1.3044E-05   6.4772E-05
2.9120E-04  -2.0469E-06  5.0986E-09   1.1369E-11  -5.9086E-08  -2.1374E-11  7.9394E-14   1.3058E-05   5.0732E-05
3.2760E-04  -1.9478E-06  5.0797E-09   1.1253E-11  -5.9044E-08  -2.1238E-11  7.9634E-14   1.3024E-05   6.1715E-05
3.6400E-04  -1.8513E-06  5.0598E-09   1.1138E-11  -5.9004E-08  -2.1110E-11  7.9857E-14   1.3017E-05   5.7810E-05
4.0040E-04  -1.7573E-06  5.0390E-09   1.1025E-11  -5.8965E-08  -2.0987E-11  8.0067E-14   1.3016E-05   5.8182E-05
4.3680E-04  -1.6659E-06  5.0175E-09   1.0914E-11  -5.8927E-08  -2.0870E-11  8.0263E-14   1.3003E-05   6.2681E-05
4.7320E-04  -1.5770E-06  4.9954E-09   1.0807E-11  -5.8892E-08  -2.0762E-11  8.0439E-14   1.2990E-05   6.2225E-05
5.0960E-04  -1.4906E-06  4.9730E-09   1.0705E-11  -5.8858E-08  -2.0658E-11  8.0603E-14   1.2985E-05   5.8033E-05
5.4600E-04  -1.4068E-06  4.9502E-09   1.0607E-11  -5.8826E-08  -2.0562E-11  8.0749E-14   1.2982E-05   5.4827E-05
5.8240E-04  -1.3393E-06  4.9273E-09   1.0515E-11  -5.8794E-08  -2.0470E-11  8.0884E-14   1.2972E-05   6.3191E-05
6.1880E-04  -1.2774E-06  4.9042E-09   1.0429E-11  -5.8764E-08  -2.0383E-11  8.1007E-14   1.2951E-05   6.3023E-05
6.5520E-04  -1.2166E-06  4.8812E-09   1.0349E-11  -5.8736E-08  -2.0305E-11  8.1112E-14   1.2939E-05   5.4712E-05
6.9160E-04  -1.1569E-06  4.8581E-09   1.0275E-11  -5.8709E-08  -2.0232E-11  8.1202E-14   1.2939E-05   5.5268E-05
7.2800E-04  -1.0517E-06  4.8167E-09   1.0152E-11  -5.8684E-08  -2.0166E-11  8.1274E-14   6.4504E-06   5.9328E-05
7.6440E-04  -9.3926E-07  4.7712E-09   1.0029E-11  -5.8662E-08  -2.0108E-11  8.1325E-14   6.4408E-06   6.3429E-05
8.0080E-04  -8.3097E-07  4.7264E-09   9.9178E-12  -5.8630E-08  -2.0032E-11  8.1381E-14   6.4260E-06   4.1247E-06
8.3720E-04  -7.2678E-07  4.6823E-09   9.8186E-12  -5.6707E-08  -1.5606E-11  8.3584E-14   6.4056E-06   5.9315E-07
8.7360E-04  -6.2669E-07  4.6392E-09   9.7308E-12  -5.5022E-08  -1.1964E-11  8.4678E-14   6.3930E-06   6.0252E-07
9.1000E-04  -5.3067E-07  4.5971E-09   9.6535E-12  -5.3437E-08  -8.7530E-12  8.4932E-14   6.3698E-06   5.4364E-07
9.4640E-04  -4.3872E-07  4.5562E-09   9.5862E-12  -5.1896E-08  -5.8331E-12  8.4478E-14   6.3534E-06   5.7109E-07
9.8280E-04  -3.5078E-07  4.5164E-09   9.5278E-12  -5.0495E-08  -3.3667E-12  8.3473E-14   6.3383E-06   5.7897E-07
1.0192E-03  -2.6687E-07  4.4780E-09   9.4774E-12  -4.8537E-08  -2.1177E-13  8.1200E-14   6.3191E-06   2.9442E-07
1.0556E-03  -1.8694E-07  4.4409E-09   9.4342E-12  -4.6253E-08   3.1782E-12  7.7831E-14   6.2973E-06   2.9978E-07
1.0920E-03  -1.1101E-07  4.4052E-09   9.3972E-12  -4.4208E-08   5.9480E-12  7.4210E-14   6.2787E-06   3.0464E-07
1.1284E-03   1.1824E-08  4.3432E-09   9.3403E-12  -4.1371E-08   9.4291E-12  6.8949E-14   3.1237E-06   1.7803E-07
1.1648E-03   1.3256E-07  4.2773E-09   9.2847E-12  -3.8655E-08   1.2276E-11  6.3080E-14   3.1034E-06   1.8187E-07
1.2012E-03   2.4153E-07  4.2142E-09   9.2344E-12  -3.6322E-08   1.4287E-11  5.7589E-14   3.2748E-06   1.7056E-07
1.2376E-03   3.0963E-07  4.1727E-09   9.2017E-12  -3.3413E-08   1.6217E-11  5.0294E-14   4.3795E-06   1.3140E-07
1.2740E-03   3.7380E-07  4.1320E-09   9.1690E-12  -2.9829E-08   1.8083E-11  4.2208E-14   4.3586E-06   7.3775E-08
1.3104E-03   4.3622E-07  4.0883E-09   9.1319E-12  -2.5925E-08   1.9617E-11  3.3972E-14   2.6852E-06   5.0134E-08
1.3468E-03   4.8983E-07  4.0346E-09   9.0833E-12  -2.1987E-08   2.0477E-11  2.6645E-14   3.0062E-06   5.5105E-08
1.3832E-03   5.3951E-07  3.9833E-09   9.0325E-12  -1.6052E-08   2.0605E-11  1.8002E-14   2.9794E-06   2.5221E-08
1.4196E-03   6.0408E-07  3.9122E-09   8.9540E-12  -9.2665E-09   2.0771E-11  1.9994E-14   1.6352E-06   1.0998E-08
1.4560E-03   6.7166E-07  3.8268E-09   8.8496E-12  -1.7335E-09   1.4986E-11  6.3826E-15   1.6093E-06   8.3872E-09
1.4924E-03   7.2047E-07  3.7442E-09   8.7367E-12   1.3855E-09   1.0386E-11  5.0619E-15   1.5822E-06   1.6600E-08
1.5288E-03   7.5151E-07  3.6569E-09   8.6033E-12   2.0654E-09   7.5683E-12  5.0176E-15   1.3969E-06   1.1062E-08
1.5652E-03   7.8286E-07  3.5534E-09   8.4275E-12   2.1173E-09   6.3249E-12  7.3221E-15   8.6138E-07   1.0959E-08
1.6016E-03   8.1039E-07  3.4255E-09   8.1902E-12   1.9029E-09   5.1754E-12  7.0594E-15   8.0830E-07   1.7031E-08
1.6380E-03   8.2883E-07  3.2568E-09   7.8509E-12   1.5273E-09   4.0916E-12  6.6201E-15   6.3009E-07   4.4101E-08
1.6744E-03   8.2553E-07  3.0381E-09   7.3789E-12   1.2379E-09   3.4008E-12  5.6295E-15   3.9312E-07   1.8817E-08
1.7108E-03   7.8406E-07  2.7555E-09   6.7380E-12   9.8825E-10   2.8033E-12  4.8645E-15   2.1001E-07   3.4422E-08
1.7472E-03   6.9967E-07  2.3832E-09   5.8641E-12   7.2883E-10   2.1427E-12  3.3813E-15   2.0701E-07   1.6967E-08
1.7836E-03   5.2223E-07  1.7770E-09   4.4038E-12   4.5398E-10   1.3876E-12  1.5784E-15   7.0525E-08   1.4391E-08
1.8200E-03   1.3642E-12 -2.2204E-16  -5.2042E-18  -8.6514E-14  -4.0779E-14 -3.1034E-15   5.8404E-13   0.0
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period of infiltration (360s) the first two terms of the series expansion, i.e. $\lambda t^{1/2}$ and $\chi_w t$ or $\chi_s t$ together contribute about 95 to 99% of the depth at which water or salt moved. As expected, the contribution of λ is between 93 to 98% at the wetting zone during the initial period of infiltration. The contribution of $\psi_w t^{3/2}$, $\psi_s t^{3/2}$, $\omega_w t^2$ and $\omega_s t^2$ to vertical downward movement of water or salt, at this initial period of infiltration, is very small, ranging from 0.16 to 4.5% for the water flow and 0.12 to 0.5% for the salt flow. The contribution of the ωt^2 term above is very small, ranging generally from 0.01 to 0.5%. For infiltration time period of about 7200s (2 hours), the contribution of λ and χ even though still dominant, diminishes slightly. At the wetting zone,the contribution of λ and χ at this time period was on the average about 92.95% and 96.87% for Akuse clay and Brookston clay, respectively. At the transition zone of moisture content $\Theta = 0.98$, however, the contribution of λ and χ had reduced to about 60.52% and 76.04% for Akuse clay and Brookston clay, respectively. The proportion contributed by ψ_w and ω_w was on the average 7.05% for Akuse clay and 3.13% for Brookston clay at the wetting zone. At the wet transition zone of $\Theta = 0.98$, however, the proportion to the total depth of water moved, contributed by ψ_w and ω_w was 39.5% and 23.96% for Akuse clay and Brookston clay, respectively. At longer time periods of 21600s (6 hours) the contribution of λ and χ is still dominant at the wetting zone (80-92%) whilst that for ψ and ω increases substantially at the wet zone of $\Theta = 0.98$ (8 to 62.5%). Note, however, that at $\Theta = 0.98$ the distance z is generally very small between 5.08×10^{-3} m for time period of 360s and 0.8 m for t=21600s, so that a contribution of 62.5% at this moisture content is very small.

TABLE 5.10a. Contribution of $\lambda t^{1/2}$, $\chi_w t$, $\psi_w t^{3/2}$ and $\omega_w t^2$ to the vertical distance moved by water (Akuse clay)

Time s	$\Theta = \frac{(\theta-\theta_n)}{(\theta_o-\theta_n)}$	Depth z m	$\lambda_t 1/2$	% Contribution to z	$\chi_w t$	% Contribution to z	$\psi_w t$	% Contribution to z	$\omega_w t^2$	% Contribution to z
360	0.05	$9.286\mathrm{x}10^{-2}$	$8.636\mathrm{x}10^{-2}$	93.00	$6.106\mathrm{x}10^{-3}$	6.57	$3.881\mathrm{x}10^{-4}$	0.42	$9.603\mathrm{x}10^{-6}$	0.01
	0.10	$9.272\mathrm{x}10^{-2}$	$8.62\ \mathrm{x}10^{-2}$	92.96	$6.128\mathrm{x}10^{-3}$	6.61	$3.872\mathrm{x}10^{-4}$	0.42	$9.682\mathrm{x}10^{-6}$	0.01
	0.50	$9.099\mathrm{x}10^{-2}$	$8.410\mathrm{x}10^{-2}$	92.43	$6.511\mathrm{x}10^{-3}$	7.16	$3.684\mathrm{x}10^{-4}$	0.41	$9.283\mathrm{x}10^{-6}$	0.01
	0.80	$8.298\mathrm{x}10^{-2}$	$7.505\mathrm{x}10^{-2}$	90.45	$7.575\mathrm{x}10^{-3}$	9.13	$3.482\mathrm{x}10^{-4}$	0.42	$1.804\mathrm{x}10^{-6}$	0.002
	0.98	$1.386\mathrm{x}10^{-2}$	$9.505\mathrm{x}10^{-3}$	68.56	$3.729\mathrm{x}10^{-3}$	26.90	$5.663\mathrm{x}10^{-4}$	4.09	$6.427\mathrm{x}10^{-5}$	0.46
7200	0.05	0.5469	0.3862	70.62	0.1221	22.33	$3.471\mathrm{x}10^{-2}$	6.35	$3.841\mathrm{x}10^{-3}$	0.70
	0.10	0.5465	0.3855	70.53	0.1226	22.42	$3.463\mathrm{x}10^{-2}$	6.34	$3.873\mathrm{x}10^{-3}$	0.71
	0.50	0.5430	0.3761	69.24	0.1302	23.98	$3.295\mathrm{x}10^{-2}$	6.07	$3.713\mathrm{x}10^{-3}$	0.68
	0.80	0.5190	0.3356	64.67	0.1515	29.19	$3.114\mathrm{x}10^{-2}$	6.00	$7.218\mathrm{x}10^{-4}$	0.14
	0.98	0.1934	$4.251\mathrm{x}10^{-2}$	21.97	$7.458\mathrm{x}10^{-2}$	38.55	$5.066\mathrm{x}10^{-2}$	26.19	$2.571\mathrm{x}10^{-2}$	13.29
14400	0.05	0.9040	0.5462	60.42	0.2442	27.01	$9.818\mathrm{x}10^{-2}$	10.86	$1.536\mathrm{x}10^{-2}$	1.70
	0.10	0.9037	0.5452	60.32	0.2451	27.12	$9.796\mathrm{x}10^{-2}$	10.84	$1.549\mathrm{x}10^{-2}$	1.71
	0.50	0.9004	0.5319	59.07	0.2605	28.93	$9.320\mathrm{x}10^{-2}$	10.35	$1.485\mathrm{x}10^{-2}$	1.65
	0.80	0.8686	0.4747	54.64	0.3030	34.88	$8.808\mathrm{x}10^{-2}$	10.14	$2.887\mathrm{x}10^{-3}$	0.33
	0.98	0.4554	$6.011\mathrm{x}10^{-2}$	13.20	0.1492	32.76	0.1433	31.46	0.1028	22.58
21600	0.05	1.2502	0.6689	53.50	0.3664	29.31	0.1804	14.43	$3.457\mathrm{x}10^{-2}$	2.77
	0.10	1.2501	0.6677	53.41	0.3677	29.41	0.1800	14.40	$3.486\mathrm{x}10^{-2}$	2.79
	0.50	1.2467	0.6514	52.25	0.3907	31.34	0.1712	13.73	$3.342\mathrm{x}10^{-2}$	2.68
	0.80	1.2042	0.5813	48.28	0.4545	37.75	0.1618	13.44	$6.496\mathrm{x}10^{-3}$	0.54
	0.98	0.7919	$7.362\mathrm{x}10^{-2}$	9.30	0.2237	28.25	0.2632	33.24	0.2314	29.22

TABLE 5.10b. Contribution of $\lambda t^{1/2}$, $\chi_s t$, $\psi_s t^{3/2}$ and $\omega_s t^2$ to the vertical distance moved by chloride (Akuse clay)

Time s	$\frac{(c-c_n)}{(c_o-c_n)}$	Depth z m	$\lambda t^{1/2}$	% Contribution to z	$\chi_s t$	% Contribution to z	$\psi_s t^{3/2}$	% Contribution to z	$\omega_s t^2$	% Contribution to z
360	0.05	$8.544x10^{-2}$	$8.028x10^{-2}$	93.96	$4.868x10^{-3}$	5.70	$2.867x10^{-4}$	0.34	$6.947x10^{-6}$	0.01
	0.10	$8.446x10^{-2}$	$7.927x10^{-2}$	93.85	$4.898x10^{-3}$	5.80	$2.874x10^{-4}$	0.34	$6.580x10^{-6}$	0.01
	0.50	$7.989x10^{-2}$	$7.469x10^{-2}$	93.49	$4.904x10^{-3}$	6.14	$2.919x10^{-4}$	0.37	$6.753x10^{-6}$	0.01
	0.80	$7.146x10^{-2}$	$6.636x10^{-2}$	92.86	$4.795x10^{-3}$	6.71	$2.989x10^{-4}$	0.42	$6.894x10^{-6}$	0.01
	0.98	$5.258x10^{-2}$	$4.832x10^{-2}$	91.91	$3.964x10^{-3}$	7.54	$2.820x10^{-4}$	0.54	$8.707x10^{-6}$	0.01
7200	0.05	0.4848	0.3590	74.67	$9.737x10^{-2}$	20.08	$2.564x10^{-2}$	5.29	$2.779x10^{-3}$	0.57
	0.10	0.4808	0.3545	73.73	$9.797x10^{-2}$	20.38	$2.571x10^{-2}$	5.35	$2.632x10^{-3}$	0.55
	0.50	0.4609	0.3340	72.47	$9.808x10^{-2}$	21.28	$2.611x10^{-2}$	5.66	$2.701x10^{-3}$	0.59
	0.80	0.4221	0.2968	70.30	$9.590x10^{-2}$	22.72	$2.674x10^{-2}$	6.33	$2.758x10^{-3}$	0.65
	0.98	0.3241	0.2161	66.68	$7.928x10^{-2}$	24.46	$2.522x10^{-2}$	7.78	$3.483x10^{-3}$	1.08
14400	0.05	0.7861	0.5077	64.59	0.1947	24.77	$7.253x10^{-2}$	9.23	$1.112x10^{-2}$	1.41
	0.10	0.7805	0.5013	64.23	0.1959	25.10	$7.272x10^{-2}$	9.23	$1.053x10^{-2}$	1.35
	0.50	0.7532	0.4724	62.72	0.1962	26.05	$7.384x10^{-2}$	9.80	$1.080x10^{-2}$	1.44
	0.80	0.6981	0.4197	60.12	0.1918	27.47	$7.562x10^{-2}$	10.83	$1.103x10^{-2}$	1.58
	0.98	0.5495	0.3056	55.62	0.1586	28.86	$7.133x10^{-2}$	12.98	$1.393x10^{-2}$	2.54
21600	0.05	1.0722	0.6219	58.00	0.2921	27.24	0.1332	12.43	$2.501x10^{-2}$	2.33
	0.10	1.0652	0.6140	57.64	0.2939	27.59	0.1336	12.54	$2.369x10^{-2}$	2.22
	0.50	1.0327	0.5785	56.02	0.2942	28.49	0.1357	13.14	$2.431x10^{-2}$	2.35
	0.80	0.9654	0.5140	53.24	0.2877	29.80	0.1389	14.39	$2.482x10^{-2}$	2.57
	0.98	0.7746	0.3743	48.33	0.2379	30.70	0.1311	16.92	$3.135x10^{-2}$	4.05

TABLE 5.11a. Contribution of $\lambda t^{1/2}$, $\chi_w t$, $\psi_w t^{3/2}$ and $\omega_w t^2$ to the vertical distance moved by water (Brookston clay)

Time s	Θ $\frac{(\theta-\theta_n)}{(\theta_o-\theta_n)}$	Depth z m	$\lambda t^{1/2}$	% Contribution to z	$\chi_w t$	% Contribution to z	$\psi_w t^{3/2}$	% Contribution to z	$\omega_w t^2$	% Contribution to z
360	0.05	3.579×10^{-2}	3.447×10^{-2}	96.32	1.259×10^{-3}	3.52	5.588×10^{-5}	0.16	1.993×10^{-6}	0.006
	0.10	3.572×10^{-2}	3.441×10^{-2}	96.34	1.252×10^{-3}	3.51	5.498×10^{-5}	0.15	1.952×10^{-6}	0.006
	0.50	3.456×10^{-2}	$3.32\ \times10^{-2}$	96.08	1.302×10^{-3}	3.77	5.161×10^{-5}	0.15	1.750×10^{-6}	0.005
	0.80	2.982×10^{-2}	2.816×10^{-2}	94.43	1.604×10^{-3}	5.38	5.693×10^{-5}	0.19	1.140×10^{-6}	0.004
	0.98	5.077×10^{-3}	4.324×10^{-3}	85.16	6.655×10^{-4}	13.11	$7.99\ \times10^{-5}$	1.57	7.841×10^{-6}	0.150
7200	0.05	0.1852	0.1542	83.27	2.519×10^{-2}	13.60	4.998×10^{-3}	2.70	7.972×10^{-4}	0.43
	0.10	0.1846	0.1539	83.35	2.505×10^{-2}	13.57	4.917×10^{-3}	2.66	7.808×10^{-4}	0.42
	0.50	0.1799	0.1485	82.57	2.604×10^{-2}	14.48	4.616×10^{-3}	2.57	7.001×10^{-4}	0.39
	0.80	0.1636	0.1259	77.00	3.207×10^{-2}	19.61	5.092×10^{-3}	3.11	4.561×10^{-4}	0.28
	0.98	4.293×10^{-2}	1.934×10^{-2}	45.04	1.331×10^{-2}	31.00	7.147×10^{-3}	16.65	3.137×10^{-3}	7.31
19260	0.05	0.3471	0.2521	72.64	6.738×10^{-2}	19.41	2.187×10^{-2}	6.30	5.704×10^{-3}	1.64
	0.10	0.3458	0.2517	72.79	6.700×10^{-2}	19.38	2.151×10^{-2}	6.22	5.587×10^{-3}	1.62
	0.50	0.3377	0.2429	71.91	6.965×10^{-2}	20.62	2.020×10^{-2}	5.98	5.010×10^{-3}	1.48
	0.80	0.3173	0.2060	64.92	8.579×10^{-2}	27.04	2.228×10^{-2}	7.02	3.264×10^{-3}	1.03
	0.98	0.1209	3.162×10^{-2}	26.15	3.560×10^{-2}	29.44	3.127×10^{-2}	25.85	2.244×10^{-3}	18.56
21600	0.05	0.3757	0.2670	71.07	7.556×10^{-2}	20.11	2.597×10^{-2}	6.91	7.175×10^{-3}	1.91
	0.10	0.3743	0.2666	71.22	7.514×10^{-2}	20.08	2.555×10^{-2}	6.83	7.028×10^{-3}	1.88
	0.50	0.3656	0.2572	70.35	7.811×10^{-2}	21.37	2.399×10^{-2}	6.56	6.301×10^{-3}	1.72
	0.80	0.3449	0.2181	63.24	9.621×10^{-2}	27.90	2.646×10^{-2}	7.67	4.105×10^{-3}	1.19
	0.98	0.1388	3.349×10^{-2}	24.13	3.993×10^{-2}	28.77	3.714×10^{-2}	26.76	2.823×10^{-2}	20.34

TABLE 5.11b. Contribution of $\lambda t^{1/2}$, $\chi_s t$, $\psi_s t^{3/2}$ and $\omega_s t^2$ to the vertical distance moved by chloride (Brookston clay)

Time s	$\frac{c-c_n}{c_o-c_n}$	Depth z m	$\lambda t^{1/2}$	% Contribution to z	$\chi_s t$	% Contribution to z	$\psi_s t^{3/2}$	% Contribution to z	$\omega_s t^2$	% Contribution to z
360	0.05	$3.125\text{x}10^{-2}$	$3.028\text{x}10^{-2}$	96.90	$9.287\text{x}10^{-4}$	2.97	$3.783\text{x}10^{-5}$	0.12	$1.240\text{x}10^{-6}$	0.004
	0.10	$3.013\text{x}10^{-2}$	$2.916\text{x}10^{-2}$	96.76	$9.375\text{x}10^{-4}$	3.11	$3.825\text{x}10^{-5}$	0.13	$1.246\text{x}10^{-6}$	0.004
	0.50	$2.805\text{x}10^{-2}$	$2.707\text{x}10^{-2}$	96.51	$9.396\text{x}10^{-4}$	3.35	$3.893\text{x}10^{-5}$	0.14	$1.255\text{x}10^{-6}$	0.005
	0.80	$2.642\text{x}10^{-2}$	$2.546\text{x}10^{-2}$	96.35	$9.229\text{x}10^{-4}$	3.49	$3.916\text{x}10^{-5}$	0.15	$1.270\text{x}10^{-6}$	0.005
	0.98	$1.959\text{x}10^{-2}$	$1.878\text{x}10^{-2}$	95.90	$7.665\text{x}10^{-4}$	3.91	$3.604\text{x}10^{-5}$	0.18	$1.290\text{x}10^{-6}$	0.007
7200	0.05	0.1579	0.1354	85.78	$1.857\text{x}10^{-2}$	11.76	$3.383\text{x}10^{-3}$	2.14	$4.962\text{x}10^{-4}$	0.31
	0.10	0.1531	0.1304	85.19	$1.875\text{x}10^{-2}$	12.25	$3.421\text{x}10^{-3}$	2.24	$4.985\text{x}10^{-4}$	0.33
	0.50	0.1439	0.1211	84.17	$1.879\text{x}10^{-2}$	13.06	$3.482\text{x}10^{-3}$	2.42	$5.021\text{x}10^{-4}$	0.35
	0.80	0.1363	0.1138	83.52	$1.846\text{x}10^{-2}$	13.54	$3.502\text{x}10^{-3}$	2.57	$5.080\text{x}10^{-4}$	0.37
	0.98	0.1031	$8.399\text{x}10^{-2}$	81.50	$1.533\text{x}10^{-2}$	14.87	$3.224\text{x}10^{-3}$	3.13	$5.161\text{x}10^{-4}$	0.50
19260	0.05	0.2895	0.2215	76.50	$4.968\text{x}10^{-2}$	17.16	$1.480\text{x}10^{-2}$	5.11	$3.551\text{x}10^{-3}$	1.23
	0.10	0.2820	0.2133	75.64	$5.016\text{x}10^{-2}$	17.79	$1.497\text{x}10^{-2}$	5.31	$3.567\text{x}10^{-3}$	1.27
	0.50	0.2671	0.1980	74.13	$5.027\text{x}10^{-2}$	18.82	$1.523\text{x}10^{-2}$	5.70	$3.593\text{x}10^{-3}$	1.35
	0.80	0.2545	0.1862	73.15	$4.937\text{x}10^{-2}$	19.40	$1.532\text{x}10^{-2}$	6.02	$3.635\text{x}10^{-3}$	1.43
	0.98	0.1962	0.1374	70.03	$4.101\text{x}10^{-2}$	20.90	$1.410\text{x}10^{-2}$	7.19	$3.693\text{x}10^{-3}$	1.88
21600	0.05	0.3123	0.2346	75.10	$5.572\text{x}10^{-2}$	17.84	$1.758\text{x}10^{-2}$	5.63	$4.466\text{x}10^{-3}$	1.43
	0.10	0.3044	0.2258	74.20	$5.625\text{x}10^{-2}$	18.48	$1.778\text{x}10^{-2}$	5.84	$4.487\text{x}10^{-3}$	1.47
	0.50	0.2887	0.2097	72.64	$5.638\text{x}10^{-2}$	19.53	$1.809\text{x}10^{-2}$	6.27	$4.519\text{x}10^{-3}$	1.57
	0.80	0.2753	0.1972	71.62	$5.537\text{x}10^{-2}$	20.11	$1.820\text{x}10^{-2}$	6.61	$4.572\text{x}10^{-3}$	1.66
	0.98	0.2129	0.1455	68.34	$4.599\text{x}10^{-2}$	21.61	$1.675\text{x}10^{-2}$	7.87	$4.645\text{x}10^{-3}$	2.18

In a preliminary test of the analysis in section 3.4 and the resultant ordinary differential equations presented in Table 3.1, computed water content profiles and computed chloride content profiles are compared with experimentally determined water content and chloride content profiles for vertical infiltration for t=7200s for Akuse clay (figures 5.21a and 5.21b) and for t=19260s for Brookston clay (figures 5.22a and 5.22b). The slight difference in theoretical and experimentally determined curves may be attributed to the slight difference in initial water content of the soils used for the horizontal infiltration experiment and those for the vertical infiltration experiments; and also to slight differences in bulk densities between soil columns used for horizontal infiltration experiments and those for vertical infiltration experiments. In spite of these problems, it is observed that there is a fairly good agreement between theoretical $z(\theta)$ and $z(c)$ profiles and the experimentally determined $z(\theta)$ and $z(c)$ data.

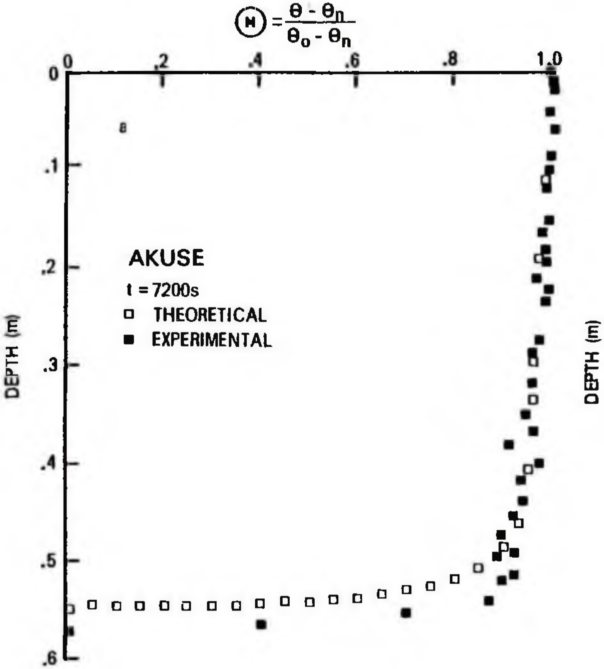
The theoretical water content profiles and chloride content profiles for various time periods for Akuse clay and Brookston clay are presented in figures 5.23a, 5.23b, 5.24a and 5.24b, respectively. It is observed that the water content profiles (figures 5.23a and 5.24a) show a sharp, abrupt wetting front whereas the chloride content profiles (figures 5.23b and 5.24b) exhibit a dispersed 'salt front'. However, the effect of gravity tends to make 'salt front' in the vertical infiltration less dispersed than the horizontal infiltration (cf. figures 5.17a, 5.17b with figures 5.23b and 5.24b). Examination of the theoretical chloride content profiles (figures 5.23b and 5.24b) reveals that the chloride content profile has a sharp front at small time periods t=360s. The front then disperses at time periods greater than the initial period.

FIGURE 5.21.

(a) Theoretical and experimental water content profiles at t=7200s (Akuse clay).

(b) Theoretical and experimental chloride content profiles at t=7200s (Akuse clay).

The theoretical curves were obtained by employing the method of Philip (1957) and the method of Elrick *et al*. (1979).



$\Theta = \frac{\theta - \theta_n}{\theta_o - \theta_n}$
0
.2
.4
.6
.8
1.0
0
.1
.2
.3
.4
.5
.6
DEPTH (m)
DEPTH (m)
AKUSE
t = 7200s
□ THEORETICAL
■ EXPERIMENTAL

Figure 5.21

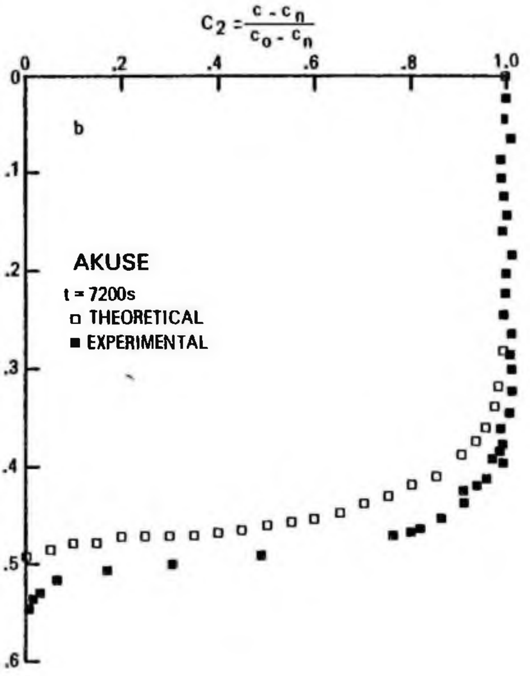

$C_2 = \frac{c - c_n}{c_o - c_n}$
0
.2
.4
.6
.8
1.0
0
.1
.2
.3
.4
.5
.6
b
AKUSE
t = 7200s
□ THEORETICAL
■ EXPERIMENTAL

FIGURE 5.22.

(a) Theoretical and experimental water content profiles at t=19260s (Brookston clay).

(b) Theoretical and experimental chloride content profiles at t=19260s (Brookston clay).

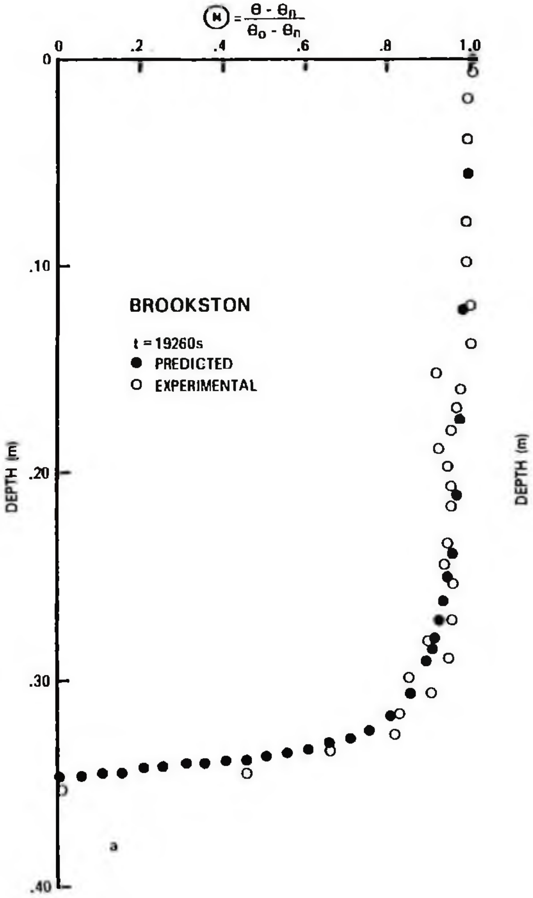

Θ = (θ - θn)/(θo - θn)
0
.2
.4
.6
.8
1.0
0
.10
.20
.30
.40
DEPTH (m)
BROOKSTON
t = 19260s
● PREDICTED
○ EXPERIMENTAL
a
DEPTH (m)

Figure 5.22

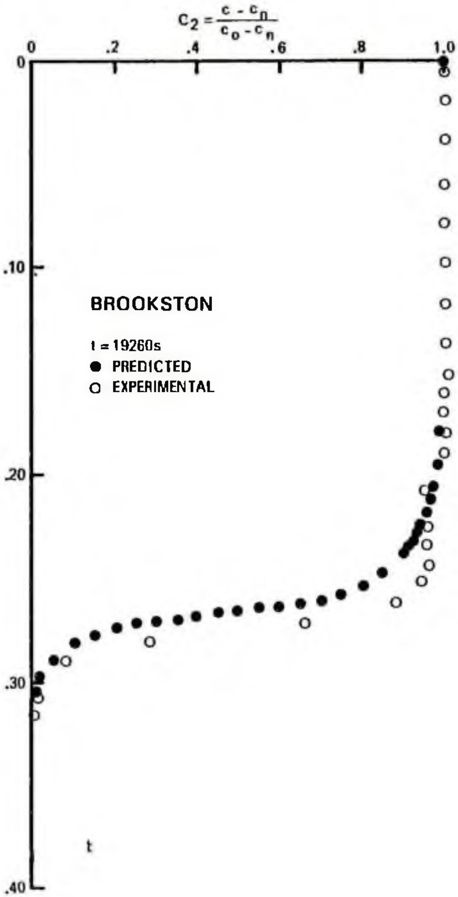
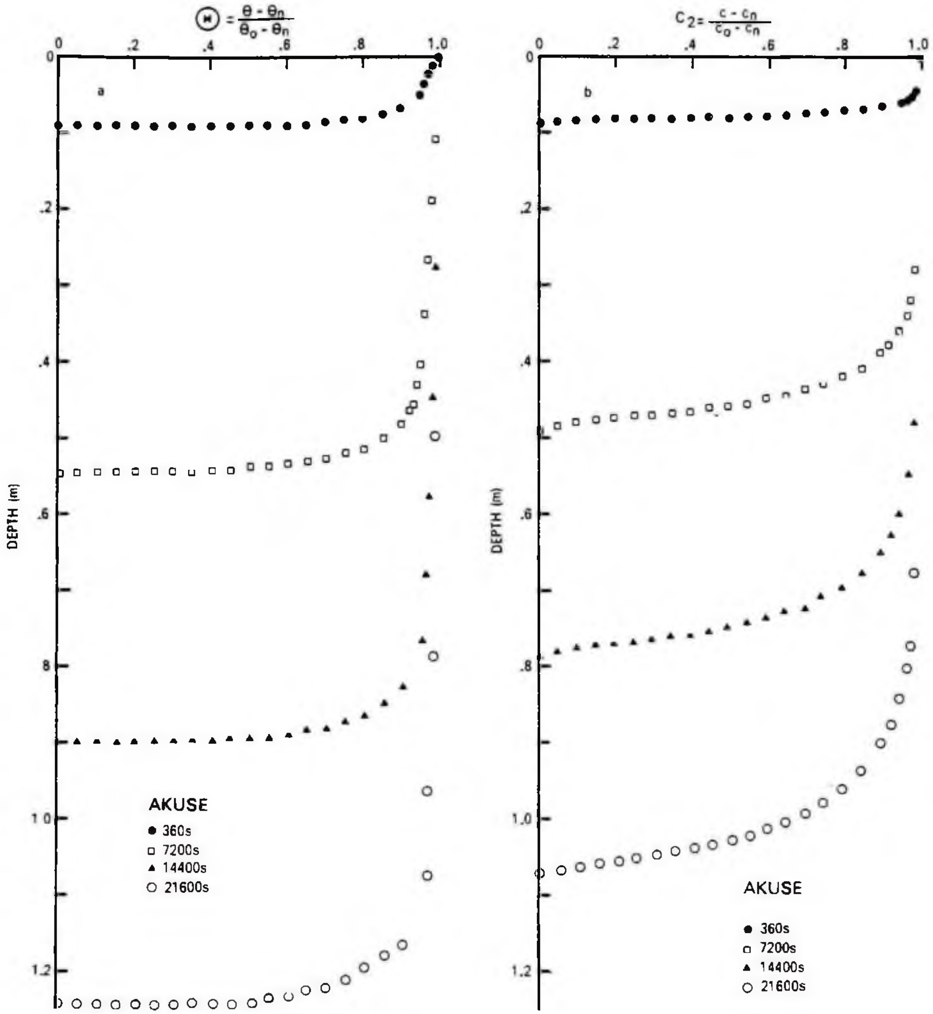

$C_2 = \frac{c - c_n}{c_o - c_n}$
0
.2
.4
.6
.8
1.0
0
.10
.20
.30
.40
BROOKSTON
t = 19260s
● PREDICTED
○ EXPERIMENTAL
t

FIGURE 5.23.

(a) Theoretical moisture content profiles for various time periods (Akuse clay).

(b) Theoretical chloride content profiles for various time periods (Akuse clay).



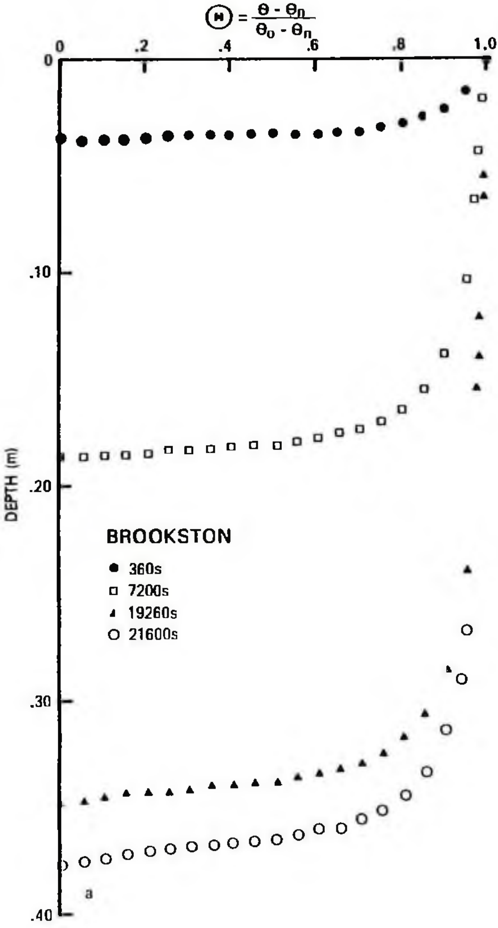
Ⓗ = (θ - θn)/(θo - θn)
0
.2
.4
.6
.8
1.0
a
DEPTH (m)
0
.2
.4
.6
.8
1.0
1.2
AKUSE
● 360s
□ 7200s
▲ 14400s
○ 21600s
C2 = (c - cn)/(co - cn)
b
DEPTH (m)
AKUSE
● 360s
□ 7200s
▲ 14400s
○ 21600s

Figure 5.23

FIGURE 5.24.

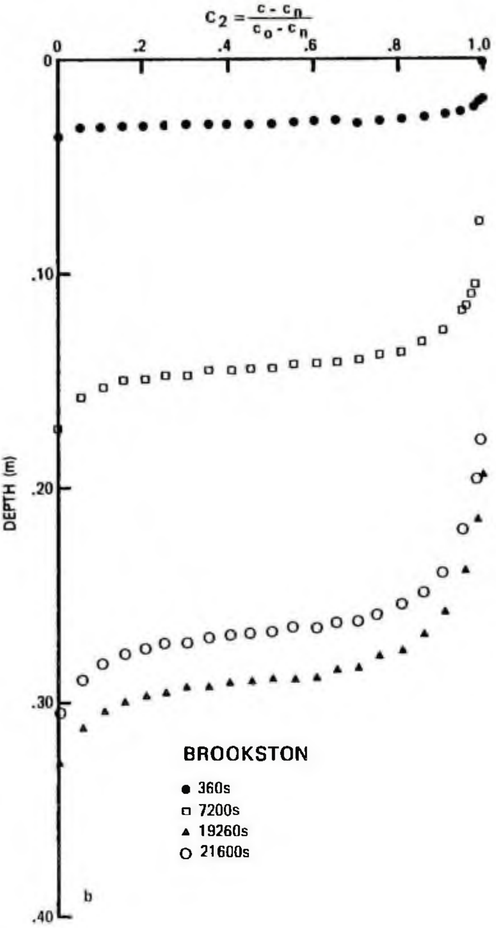
(a) Theoretical water content profiles for various time periods (Brookston clay).

(b) Theoretical chloride content profiles for various time periods (Brookston clay).



$\Theta = \frac{\theta - \theta_n}{\theta_0 - \theta_n}$
0
.2
.4
.6
.8
1.0
0
.10
.20
.30
.40
DEPTH (m)
BROOKSTON
● 360s
□ 7200s
▲ 19260s
○ 21600s
a

Figure 5.24


$C_2 = \frac{c - c_n}{c_0 - c_n}$
0
.2
.4
.6
.8
1.0
0
.10
.20
.30
.40
DEPTH (m)
BROOKSTON
● 360s
□ 7200s
▲ 19260s
○ 21600s
b

CHAPTER 6

CONCLUSIONS

In this study, simultaneous transport of water and solutes during one dimensional horizontal and vertical infiltration has been examined from the point of view of experimentation, mathematical analysis presented by Smiles *et al*. (1978), Smiles and Philip (1978) and Elrick *et al*. (1979), and simulation of the water and chloride content profiles using CSMP. Porous media, especially soils, are extremely complex and for a given solute species of interest in a given system, many physical and/or chemical processes can occur simultaneously, greatly complicating the analysis. Such processes include adsorption or ion exchange, various chemical and physical reactions, precipitation, anion exclusion and dispersion. Of these, dispersion, anion exclusion, adsorption or ion exchange processes have been dealt with in this study.

The one-dimensional horizontal infiltration experiments with KCl solution conducted in this study have shown that the water, the chloride and the potassium concentration profiles preserved similarity in terms of the distance divided by square root of time. This observation, reported earlier by Scotter and Raats (1970) for studies with NaCl, has recently been confirmed by the studies of Smiles *et al*. (1978) and Smiles and Philip (1978). The experimental results and the foregoing analysis in this study also lead to the conclusion that the transport of KCl during unsaturated flow in the soils studied, may be described by a velocity-independent dispersion coefficient. This conclusion is consistent with the studies of Saffman (1959), Pfannkuch (1963), Smiles et al. (1978), and Smiles and Philip (1978) and represents a very good simplification of the formulation, analysis and prediction of solute transport in such systems.

It is observed in this study that the chloride concentration 'front' lags behind the infiltration front. This partial piston-like displacement of the initial water content of the soil column by the encroaching KCl solution was also observed by Warrick et al. (1971), Kirda et al. (1973, 1974), Smiles et al. (1978) and Smiles and Philip (1978). The conclusion by Smiles and Philip (1978) that the whole initial water content is swept in its entirety by the encroaching KCl solution, however, was not observed in this study.

The observed effect of salt exclusion in Akuse soil whose clay fraction is almost entirely made up of smectite (Acquaye, 1973) is quite significant. Similar observations regarding anion exclusion have been made by Thomas and Swoboda (1970) and Warrick et al. (1971). The theoretical analysis presented in this study is adequate to obtain positive D_s values provided the concentration of all salts in solution has been measured. Further experimental studies into this aspect of solute movement is necessary.

The soils studied show that equilibrium adsorption isotherms for these two soils describe the adsorption phenomenon fairly well as observed from the agreement of D_s values obtained for Cl^- and for K^+. This is consistent with the observation by van Genutchen et al. (1974) that at low pore water velocities the equilibrium model for adsorption isotherm describes the adsorption phenomenon adequately.

The computer programs presented in this study, especially the algorithm, are very useful and predict very well, the soil water content, concentration of Cl^- in solution and concentration of K^+ in solution as functions of distance divided by the square root of time. In the case of Cl^-, the $c(\lambda)$ relationship computed with both the analytical solution and the non-analytical solution provided by the algorithm, agree very well with experimentally determined $c(\lambda)$ data. Provided with $D_s(\theta)$ and $D(\theta)$ or $D_s(\lambda)$ and $D(\lambda)$, the water content and concentration of Cl^- as a function of $\lambda(=x/\sqrt{t})$ can be simulated to a good degree of accuracy using the computer programs described in this study.

The analysis developed by Smiles et al. (1978) to describe hydrodynamic dispersion during one-dimensional infiltration of a solution into soil which was extended by Elrick et al. (1979) to describe one-dimensional vertical infiltration, has been used in this study to show that the power series solution in $t^{1/2}$ for concentration, similar to that developed by Philip (1957) for water, is a powerful mathematical tool for describing both water and salt content profiles during vertical infiltration of water and salt into a soil with constant initial water and salt content. Theoretical data for both water and chloride content profiles agree fairly well with experimental data. This approach developed by Elrick et al. (1979) presents a new way of describing simultaneous movement of water and solutes in soils under conditions of changing water contents and fits more closely the natural conditions encountered in the field. Theoretical water content profiles show a transition zone of uniform water content and an abrupt, sharp wetting front of low water content. This abrupt, sharp wetting front is also observed visually during the experiments and has been reported earlier by other workers like Bodman and Colman (1944), Youngs (1957) and Childs (1964). The theoretical chloride content profiles, however, show a dispersed 'salt front'.

The experimentally determined λ and the calculated χ, ψ and ω were of the order of magnitude 10^{-3}, 10^{-5}, 10^{-8} and 10^{-10}, respectively, for Akuse clay and 10^{-3}, 10^{-6}, 10^{-8} and 10^{-11}, respectively, for Brookston clay. This is an indication that the dominant terms in the series expansion are λ and χ. Derived data for the percent contribution of each of the terms $\lambda t^{1/2}$, χt, $\psi t^{3/2}$ and ωt^2 to the distance moved vertically downward by both water and chloride leads to the conclusion that at the onset and during the early stages of infiltration the dominant terms are $\lambda t^{1/2}$ and χt which together contribute between 95 to 99% of the depth at which water or salt moved. At longer duration of infiltration, the $\lambda t^{1/2}$ and χt terms, even though still dominant at the wetting zone, diminish slightly and contribute on the average about 80 to 92% to the depth at which water or salt moved at the wetting zone.

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APPENDICES

APPENDIX A

Development of the ordinary differential equations for χ, ψ, ω as given by Philip (1957)

Following Philip's (1957) notation, the horizontal space coordinate in equation 3.11a will be assigned x' and the vertical coordinate of equation 3.53 given x instead of z. The identity:

$$\left[\frac{\partial\theta}{\partial t}\right]_x \cdot \left[\frac{\partial x}{\partial\theta}\right]_t = -\left[\frac{\partial x}{\partial t}\right]_\theta \tag{A1}$$

is introduced to make x' and x (equations 3.11a and 3.53 with x' and x for space coordinates respectively) the dependent variables giving:

$$-\frac{\partial x}{\partial t} = \frac{\partial}{\partial\theta}\left[D(\theta)\,\frac{\partial\theta}{\partial x}\right] - \frac{\partial K(\theta)}{\partial\theta} \tag{A2}$$

$$-\frac{\partial x'}{\partial t} = \frac{\partial}{\partial\theta}\left[D(\theta)\,\frac{\partial\theta}{\partial x'}\right] \tag{A3}$$

Subtraction of A3 from A2 gives

$$-\frac{\partial}{\partial t}(x-x') = \frac{\partial}{\partial\theta}\left[D\left\{\frac{1}{\partial x/\partial\theta} - \frac{1}{\partial x'/\partial\theta}\right\}\right] - \frac{\partial K}{\partial\theta}$$

which may further be algebraically rearranged to obtain

$$-\frac{\partial}{\partial t}(x-x') = \frac{\partial}{\partial\theta}\left[D\left\{\frac{\partial x'/\partial\theta-\partial x/\partial\theta}{(\partial x/\partial\theta)(\partial x'/\partial\theta)}\right\}\right] - \frac{\partial K}{\partial\theta}$$

$$= \frac{\partial}{\partial\theta}\left[-D\left\{\frac{\frac{\partial}{\partial\theta}(x-x')}{(\partial x/\partial\theta)(\partial x'/\partial\theta)}\right\}\right] - \frac{\partial K}{\partial\theta}$$

Substitution of y = x-x' yields

$$-\frac{\partial y}{\partial t} = \frac{\partial}{\partial\theta}\,[-D\,\frac{\partial y/\partial\theta}{(\partial x/\partial\theta)(\partial x'/\partial\theta}\,] - \frac{\partial K}{\partial\theta}$$

Therefore,

$$-\frac{\partial y}{\partial t} = \frac{\partial}{\partial\theta}\,[-D\,\frac{\partial y}{\partial\theta}\,\frac{\partial\theta}{\partial x}\,\frac{\partial\theta}{\partial x'}\,] - \frac{\partial K}{\partial\theta} \qquad \text{(A4)}$$

Note: $\frac{\partial\theta}{\partial x} - \frac{\partial\theta}{\partial x'} = -\frac{\partial y}{\partial\theta}\,\frac{\partial\theta}{\partial x}\,\frac{\partial\theta}{\partial x'}$ (A5)

Approximation 1: Let $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial x'}$ and so y = y'

Equation A4 becomes:

$$-\frac{\partial y'}{\partial t} = \frac{\partial}{\partial\theta}\,[-D(\frac{\partial\theta}{\partial x'})^2\,\frac{\partial y'}{\partial\theta}\,] - \frac{\partial K}{\partial\theta} \qquad \text{(A6)}$$

Let $x'=\lambda t^{1/2}$; therefore $\partial x'/\partial\lambda = t^{1/2}$

$$\frac{\partial y'}{\partial t} = \frac{\partial}{\partial\theta}\,[\frac{D}{t}\,(\frac{\partial\theta}{\partial\lambda})^2\frac{\partial y'}{\partial\theta}\,] + \frac{\partial K}{\partial\theta} \qquad \text{(A7)}$$

Ordinary differential equation for χ:

Let $\chi = y't^{-1}$

Therefore,

$$\frac{\partial y'}{\partial t} = \chi \qquad \text{and} \qquad \frac{\partial y'}{\partial\chi} = t \qquad \text{(A8)}$$

Substitute A8 into A7

$$\chi = \frac{\partial}{\partial\theta}\left[\frac{D}{t}\left(\frac{\partial\theta}{\partial\lambda}\right)^2 \frac{\partial y'}{\partial\chi}\,\frac{\partial\chi}{\partial\theta}\right] + \frac{\partial K}{\partial\theta}$$

$$= \frac{\partial}{\partial\theta}\left[\frac{D}{t}\left(\frac{\partial\theta}{\partial\lambda}\right)^2 \frac{\partial\chi}{\partial\theta}\, t\right] + \frac{\partial K}{\partial\theta}$$

$$= \frac{d}{d\theta}\left[D\left(\frac{d\theta}{d\lambda}\right)^2 \frac{d\chi}{d\theta}\right] + \frac{dK}{d\theta}$$

Therefore,

$$\chi = \frac{d}{d\theta}\left[P(\theta)\,\frac{d\chi}{d\theta}\right] + \frac{dK}{d\theta} \qquad (A9)$$

where $P(\theta) = D(\theta)\ \left(\frac{d\theta}{d\lambda}\right)^2$ (A10)

Ordinary differential equation for ψ:

Starting from equations A4 and A6, subtract A6 from A4 to get:

$$-\frac{\partial}{\partial t}(y-y') = -\frac{\partial}{\partial\theta}\left[D\left\{\frac{\partial y}{\partial\theta}\,\frac{\partial\theta}{\partial x}\,\frac{\partial\theta}{\partial x'} - \left(\frac{\partial\theta}{\partial x'}\right)^2 \frac{\partial y'}{\partial\theta}\right\}\right] \qquad (A11)$$

Let $z = y-y'$.

$$\frac{\partial z}{\partial t} = \frac{\partial}{\partial\theta}\left[D\,\frac{\partial\theta}{\partial x'}\left\{\frac{\partial y}{\partial x} - \frac{\partial\theta}{\partial x'}\,\frac{\partial y'}{\partial\theta}\right\}\right]$$

$$\frac{\partial z}{\partial t} = \frac{\partial}{\partial\theta}\left[D\,\frac{\partial\theta}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right)\right] \qquad (A12)$$

$(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'})$ on the righthand side of equation A12 is expanded algebraically as follows:

$$\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'} = \frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x} + \frac{\partial y'}{\partial x} - \frac{\partial y'}{\partial x'}$$

$$= \frac{\partial z}{\partial x} + \frac{\partial y'}{\partial x} - \frac{\partial y'}{\partial x'} \quad \text{since} \quad \frac{\partial z}{\partial x} = \frac{\partial(y-y')}{\partial x} = \frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x}$$

$$= \frac{\partial z}{\partial x} + \frac{\partial y'}{\partial x'}\frac{\partial x'}{\partial x} - \frac{\partial y'}{\partial x'}$$

$$= \frac{\partial z}{\partial x} + \frac{\partial y'}{\partial x'}(\frac{\partial x'}{\partial x} - 1)$$

Since $(\frac{\partial x'}{\partial x} - 1) = (\frac{\partial x'}{\partial x} - \frac{\partial x}{\partial x}) = \frac{\partial(x'-x)}{\partial x} = -\frac{\partial y}{\partial x}$,

$$\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'} = \frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} \tag{A13}$$

Substitute A13 into A12 to obtain

$$\frac{\partial z}{\partial t} = \frac{\partial}{\partial \theta}[D \frac{\partial \theta}{\partial x'} \{ \frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} \}] \tag{A14}$$

Approximation 2: Let $\frac{\partial z}{\partial x} = \frac{\partial z'}{\partial x'}$, $\frac{\partial y}{\partial x} = \frac{\partial y'}{\partial x'}$, $z = z'$

Equation A14 then becomes:

$$\frac{\partial z'}{\partial t} = \frac{\partial}{\partial \theta}[D \frac{\partial \theta}{\partial x'} \{ \frac{\partial z'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2 \}] \tag{A15}$$

Now, $x' = \lambda t^{1/2}$, $y' = \chi t$, $P = D(\frac{d\theta}{d\lambda})^2$

$$\frac{\partial\theta}{\partial x'} = \frac{\partial\theta}{\partial\lambda}\,\frac{\partial\lambda}{\partial x'} = \frac{1}{t^{1/2}}\,\frac{d\theta}{d\lambda} \qquad \text{(A16)}$$

$$\frac{\partial\theta}{\partial y'} = \frac{d\theta}{d\chi}\,\frac{\partial\chi}{\partial y'} = \frac{1}{t}\,\frac{d\theta}{d\chi} \qquad \text{(A17)}$$

$$\frac{\partial y'}{\partial x'} = \frac{\partial y}{\partial\theta}\,\frac{\partial\theta}{\partial x'} = t\,\frac{d\chi}{d\theta}\,\frac{1}{t^{1/2}}\,\frac{d\theta}{d\lambda} = t^{1/2}\,\frac{d\chi}{d\lambda} \qquad \text{(A18)}$$

Substitute A16, A17, A18 into A15 to obtain:

$$\frac{\partial z'}{\partial t} = \frac{\partial}{\partial\theta}\left[\frac{D}{t^{1/2}}\,\frac{d\theta}{d\lambda}\left\{\frac{\partial z'}{\partial\theta}\,\frac{\partial\theta}{\partial x'} - t\left(\frac{d\chi}{d\lambda}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial\theta}\left[\frac{D}{t^{1/2}}\,\frac{d\theta}{d\lambda}\left\{\frac{1}{t^{1/2}}\,\frac{d\theta}{d\lambda}\,\frac{\partial z'}{\partial\theta} - t\left(\frac{d\chi}{d\lambda}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial\theta}\left[\frac{D}{t}\left(\frac{d\theta}{d\lambda}\right)^2\frac{\partial z'}{\partial\theta} - t^{1/2}D\,\frac{d\theta}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2\right]$$

Therefore,

$$\frac{\partial z'}{\partial t} = \frac{\partial}{\partial\theta}\left[\frac{P}{t}\,\frac{\partial z'}{\partial\theta} - t^{1/2}\,Q\right] \qquad \text{(A19)}$$

Where $Q(\theta) = D(\theta)\,\frac{d\theta}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2$

Let $\psi = \frac{z'}{t^{3/2}}$; therefore, $z' = \psi t^{3/2}$ and $\frac{\partial z'}{\partial t} = \frac{3}{2}\psi t^{1/2}$

Also, $\frac{\partial z'}{\partial\theta} = \frac{\partial z'}{\partial\psi}\,\frac{d\psi}{d\theta} = t^{3/2}\,\frac{d\psi}{d\theta}$

which upon substitution into A19 yields:

$$\frac{3}{2}\,\psi t^{1/2} = \frac{\partial}{\partial\theta}\left[\frac{P}{t}\,t^{3/2}\,\frac{d\psi}{d\theta} - t^{1/2}\,Q\right]$$

Therefore,

$$\frac{3}{2}\,\psi = \frac{d}{d\theta}\left[P(\theta)\,\frac{d\psi}{d\theta} - Q(\theta)\right] \qquad \text{(A20)}$$

Ordinary differential equation for ω :

Start with equations A14 and A15. A15 is subtracted from A14 to obtain

$$\frac{\partial}{\partial t}(z-z') = \frac{\partial}{\partial\theta}\left[D\,\frac{\partial\theta}{\partial x'}\left\{\left(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}\right) - \left(\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right)\right\}\right]$$

Let $w = z-z'$

$$\frac{\partial w}{\partial t} = \frac{\partial}{\partial\theta}\left[D\,\frac{\partial\theta}{\partial x'}\left\{\left(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}\right) - \left(\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right)\right\}\right] \qquad \text{(A21)}$$

$\left(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}\right)$ in equation A21 may be rearranged as:

$$\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'} = \frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x} + \frac{\partial z'}{\partial x} - \frac{\partial z'}{\partial x'}$$

$$= \frac{\partial w}{\partial x} + \frac{\partial z'}{\partial x'}\,\frac{\partial x'}{\partial x} - \frac{\partial z'}{\partial x'}$$

$$= \frac{\partial w}{\partial x} + \frac{\partial z'}{\partial x'}\left(\frac{\partial x'}{\partial x} - 1\right)$$

Since $\frac{\partial x'}{\partial x} - 1 = \frac{\partial x'}{\partial x} - \frac{\partial x}{\partial x} = \frac{\partial(x'-x)}{\partial x} = -\frac{\partial y}{\partial x}$

$$\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'} = \frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'}\frac{\partial y}{\partial x} \qquad \text{(A22)}$$

Substitute A22 into A21 to get:

$$\frac{\partial w}{\partial t} = \frac{\partial}{\partial \theta}\left[D\frac{\partial \theta}{\partial x'}\left\{\left(\frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'}\frac{\partial y}{\partial x}\right) - \left(\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right)\right\}\right] \qquad \text{(A23)}$$

$\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2$ in equation A23 is rearranged as:

$$\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2 = \frac{\partial y'}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right)$$

Because $y = x-x'$ and $z = y-y'$,

$y = z+y'$ and $\frac{\partial y}{\partial x} = \frac{\partial z}{\partial x} + \frac{\partial y'}{\partial x}$

Therefore,

$$\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2 = \frac{\partial y'}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right) = \frac{\partial y'}{\partial x'}\left(\frac{\partial z}{\partial x} + \frac{\partial y'}{\partial x} - \frac{\partial y'}{\partial x'}\right)$$

And so,

$$\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2 = \frac{\partial y'}{\partial x'}\left(\frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'}\right) \qquad \text{(A24)}$$

Since $\frac{\partial y'}{\partial x} - \frac{\partial y'}{\partial x'} = \frac{\partial x'}{\partial x}\frac{\partial y'}{\partial x'} - \frac{\partial y'}{\partial x'}$

$$= \frac{\partial y'}{\partial x'}\left(\frac{\partial x'}{\partial x} - 1\right)$$

$$= \frac{\partial y'}{\partial x'} \frac{\partial (x'-x)}{\partial x}$$

$$= - \frac{\partial y'}{\partial x'} \frac{\partial y}{\partial x}$$

Substitute A24 into A23 to obtain

$$\frac{\partial w}{\partial t} = \frac{\partial}{\partial \theta} [D \frac{\partial \theta}{\partial x'} \{ (\frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'} \frac{\partial y}{\partial x}) - \frac{\partial y'}{\partial x'} (\frac{\partial z}{\partial x} - \frac{\partial y}{\partial x} \frac{\partial y'}{\partial x'}) \}]$$

Approximation 3:

Let $\frac{\partial w}{\partial x} = \frac{\partial w'}{\partial x'}$, $\frac{\partial y}{\partial x} = \frac{\partial y'}{\partial x'}$, $\frac{\partial z}{\partial x} = \frac{\partial z'}{\partial x'}$ and $\frac{\partial w}{\partial t} = \frac{\partial w'}{\partial t}$

Therefore:

$$\frac{\partial w'}{\partial t} = \frac{\partial}{\partial \theta} [D \frac{\partial \theta}{\partial x'} \{ (\frac{\partial w'}{\partial x'} - \frac{\partial z'}{\partial x'} \frac{\partial y'}{\partial x'} - \frac{\partial y'}{\partial x'} (\frac{\partial z'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2 \}] \qquad (A25)$$

Now, $x' = \lambda t^{1/2}$, $y' = \chi t$, $z' = \psi t^{3/2}$

Therefore,

$$\frac{\partial z'}{\partial x'} = \frac{\partial z'}{\partial \theta} \frac{\partial \theta}{\partial x'} = t^{3/2} \frac{d\psi}{d\theta} \frac{1}{t^{1/2}} \frac{d\theta}{d\lambda} = t \frac{d\psi}{d\lambda} \qquad (A26)$$

$$\frac{\partial w'}{\partial x'} = \frac{\partial w'}{\partial \theta} \frac{\partial \theta}{\partial x'} = \frac{1}{t^{1/2}} \frac{\partial w'}{\partial \theta} \frac{\partial \theta}{\partial \lambda} \qquad (A27)$$

and

$$\frac{\partial y'}{\partial x'} = \frac{t}{t^{1/2}} \frac{d\chi}{d\lambda} = t^{1/2} \frac{d\chi}{d\lambda} \qquad (A28)$$

Substitute A26, A27, A28 into A25

$$\frac{\partial w'}{\partial t} = \frac{\partial}{\partial \theta} [\frac{1}{t^{1/2}} D \frac{d\theta}{d\lambda} \{ \frac{1}{t^{1/2}} \frac{\partial w'}{\partial \theta} \frac{\partial \theta}{\partial \lambda} - t \frac{d\psi}{d\lambda} t^{1/2} \frac{d\chi}{d\lambda}$$

$$- t^{1/2} \frac{d\chi}{d\lambda} (t \frac{d\psi}{d\lambda} - t(\frac{d\chi}{d\lambda})^2) \}]$$

$$\frac{\partial w'}{\partial t} = \frac{\partial}{\partial \theta} [\frac{D}{t} (\frac{d\theta}{d\lambda})^2 \frac{\partial w'}{\partial \theta} - 2tD \frac{d\theta}{d\lambda} \frac{d\psi}{d\lambda} \frac{d\chi}{d\lambda} + tD \frac{d\theta}{d\lambda} (\frac{d\chi}{d\lambda})^3] \qquad (A29)$$

$$\frac{\partial w'}{\partial t} = \frac{\partial}{\partial \theta} [\frac{P}{t} \frac{\partial w'}{\partial \theta} - tD \frac{d\theta}{d\lambda} \frac{d\chi}{d\lambda} \{ 2 \frac{d\psi}{d\lambda} - (\frac{d\chi}{d\lambda})^2 \}] \qquad (A30)$$

Letting $R(\theta) = D(\theta) \frac{d\theta}{d\lambda} \frac{d\chi}{d\lambda} [2 \frac{d\psi}{d\lambda} - (\frac{d\chi}{d\lambda})^2]$,

equation A30 becomes:

$$\frac{\partial w'}{\partial t} = \frac{\partial}{\partial \theta} [\frac{P}{t} \frac{\partial w'}{\partial \theta} - tR] \qquad (A31)$$

Let $\omega = \frac{w'}{t^2}$ $\qquad \frac{\partial w'}{\partial t} = 2\omega t$

Also, $\frac{\partial w'}{\partial \theta} = \frac{\partial w'}{\partial \omega} \frac{\partial \omega}{\partial \theta} = t^2 \frac{d\omega}{d\theta}$

Equation A31 becomes:

$$2\omega t = \frac{\partial}{\partial \theta} [\frac{P}{t} t^2 \frac{d\omega}{d\theta} - tR]$$

Therefore, $2\omega = \frac{d}{d\theta} [P(\theta) \frac{d\omega}{d\theta} - R(\theta)]$ $\qquad$ (A32)

APPENDIX B

Development of the ordinary differential equations for χ, ψ, ω for salt movement as given by Elrick *et al.* (1979)

The procedure developed by Elrick *et al.* (1979) for vertical flow of salt parallels very closely the development by Philip (1957) for water flow given in Appendix A. The identity (refer to equation A1) used previously is employed to transform equations 3.55 and 3.15a so that x' and x become the dependent variable as follows:

$$-\theta \frac{\partial x}{\partial t}\frac{\partial c}{\partial x} = \frac{\partial}{\partial c}\left[\frac{\theta D_s}{\partial x/\partial c}\right]\frac{\partial c}{\partial x} + D(\theta)\frac{\partial \theta}{\partial x}\frac{\partial c}{\partial x} - K\frac{\partial c}{\partial x}$$

$$\theta\frac{\partial x}{\partial t} + \frac{D(\theta)}{\partial x/\partial \theta} - K = -\frac{\partial}{\partial c}\left[\frac{\theta D_s}{\partial x/\partial c}\right] \qquad \text{(B1)}$$

and

$$-\theta \frac{\partial x'}{\partial t}\frac{\partial c}{\partial x'} = \frac{\partial}{\partial c}\left[\frac{\theta D_s}{\partial x'/\partial c}\right]\frac{\partial c}{\partial x'} + D\frac{\partial \theta}{\partial x'}\frac{\partial c}{\partial x'}$$

$$\theta\frac{\partial x'}{\partial t} + \frac{D(\theta)}{\partial x'/\partial \theta} = -\frac{\partial}{\partial c}\left[\frac{\theta D_s}{\partial x'/\partial c}\right] \qquad \text{(B2)}$$

Subtraction of B2 from B1 and substitution of

$y = x-x'$ yields

$$\theta\frac{\partial y}{\partial t} - D\frac{\partial \theta}{\partial x'}\frac{\partial y}{\partial x} - K = \frac{\partial}{\partial c}\left[\theta D_s\frac{\partial c}{\partial x'}\frac{\partial y}{\partial x}\right] \qquad \text{(B3)}$$

It must be mentioned that as was done in Appendix A,

$$-\frac{\partial\theta}{\partial x'}\,\frac{\partial y}{\partial x} = -\frac{\partial\theta}{\partial x'} + \frac{\partial\theta}{\partial x'}\,\frac{\partial x'}{\partial x} = \frac{\partial\theta}{\partial x} - \frac{\partial\theta}{\partial x'} \qquad \text{(B4)}$$

Approximation 1:

Let $\frac{\partial y}{\partial x} = \frac{\partial y'}{\partial x'}$ and $y=y'$

The second term on the lefthand side of equation B3 becomes

$$D\,\frac{\partial\theta}{\partial x'}\,\frac{\partial y}{\partial x} = D\,\frac{\partial\theta}{\partial x'}\,\frac{\partial y'}{\partial x'} = D\,\frac{\partial\theta}{\partial x'}\,\frac{\partial y'}{\partial\theta}\,\frac{\partial\theta}{\partial x'} = D\left(\frac{\partial\theta}{\partial x'}\right)^2\frac{\partial y'}{\partial\theta} \qquad \text{(B5)}$$

The term on the righthand side is also rearranged as

$$\frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\,\frac{\partial y}{\partial x}\right] = \frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\,\frac{\partial y'}{\partial c}\,\frac{\partial c}{\partial x'}\right] = \frac{\partial}{\partial c}\left[\theta D_s\left(\frac{\partial c}{\partial x'}\right)^2\frac{\partial y'}{\partial c}\right] \qquad \text{(B6)}$$

so that substitution of B5 and B6 into B3 yields

$$\theta\,\frac{\partial y'}{\partial t} - D\left(\frac{\partial\theta}{\partial x'}\right)^2\frac{\partial y'}{\partial\theta} - K = \frac{\partial}{\partial c}\left[\theta D_s\left(\frac{\partial c}{\partial x'}\right)^2\frac{\partial y'}{\partial c}\right] \qquad \text{(B7)}$$

Now, let $x'=\lambda t^{1/2}$, $P(\theta) = D(\theta)\left(\frac{d\theta}{d\lambda}\right)^2$

Therefore,

$$\frac{\partial\theta}{\partial x'} = \frac{d\theta}{d\lambda}\,\frac{\partial\lambda}{\partial x'} = \frac{d\theta}{d\lambda}\,\frac{1}{t^{1/2}}$$

Equation B7 therefore becomes:

$$\theta\frac{\partial y'}{\partial t} - \frac{1}{t}D\left(\frac{d\theta}{d\lambda}\right)^2\frac{\partial y'}{\partial \theta} - K = \frac{\partial}{\partial c}\left[\theta D_s\left(\frac{dc}{d\lambda}\right)^2\frac{1}{t}\frac{\partial y'}{\partial c}\right]$$

$$\theta\frac{\partial y'}{\partial t} - \frac{P(\theta)}{t}\frac{\partial y'}{\partial \theta} - K = \frac{1}{t}\frac{\partial}{\partial c}\left[P_s(\theta)\frac{\partial y'}{\partial c}\right] \tag{B8}$$

where $P_s(\theta) = \theta D_s\left(\frac{dc}{d\lambda}\right)^2$

Ordinary differential equation for χ:

Let $\chi = \frac{y'}{t}$. Therefore, $\frac{\partial y'}{\partial t} = \chi$, $\frac{\partial y'}{\partial \theta} = t\frac{d\chi}{d\theta}$ and $\frac{\partial y'}{\partial c} = t\frac{d\chi}{dc}$

Therefore, equation B8 becomes

$$\theta\chi - \frac{P(\theta)}{t}\,t\frac{d\chi}{d\theta} - K(\theta) = \frac{1}{t}\frac{d}{dc}\left[P_s\,t\frac{d\chi}{dc}\right]$$

$$\theta\chi - P(\theta)\frac{d\chi}{d\theta} - K(\theta) = \frac{d}{dc}\left[P_s(\theta)\frac{d\chi}{dc}\right] \tag{B9}$$

Ordinary differential equation for ψ:

We start with equation B3 and B7.

Noting that $D\left(\frac{\partial\theta}{\partial x'}\right)^2\frac{\partial y'}{\partial\theta}$ in equation B7 may be rewritten as

$$D\frac{\partial\theta}{\partial x'}\frac{\partial\theta}{\partial x'}\frac{\partial y'}{\partial\theta} = D\frac{\partial\theta}{\partial x'}\frac{\partial y'}{\partial x'}$$ and also,

$$\theta D_s\left(\frac{\partial c}{\partial x'}\right)^2\frac{\partial y'}{\partial c} = \theta D_s\frac{\partial c}{\partial x'}\frac{\partial c}{\partial x'}\frac{\partial y'}{\partial c} = \theta D_s\frac{\partial c}{\partial x'}\frac{\partial y'}{\partial x'}$$

equation B7 is subtracted from B3 to obtain

$$\theta\frac{\partial(y-y')}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right) = \frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right)\right] \qquad (B10)$$

Let $z = y-y'$

Therefore,

$$\theta\frac{\partial z}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right) = \frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right)\right] \qquad (B11)$$

$$\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'} = \frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'}$$ (refer to equation A13)

Therefore,

$$\theta\frac{\partial z}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\left[\frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'}\right] = \frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\left(\frac{\partial z}{\partial x} - \frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'}\right)\right] \qquad (B12)$$

Approximation 2:

Let $\frac{\partial z}{\partial x} = \frac{\partial z'}{\partial x'}$, $\frac{\partial y}{\partial x} = \frac{\partial y'}{\partial x'}$ and $z=z'$

Equation B12 becomes:

$$\theta\frac{\partial z'}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\left[\frac{\partial z'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right] = \frac{\partial}{\partial c}\left[\theta D_s\,\frac{\partial c}{\partial x'}\left(\frac{\partial z'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right)\right] \qquad (B13)$$

Now $x' = \lambda t^{1/2}$, $y' = \chi t$, $P(\theta) = D(\theta)\left(\frac{d\theta}{d\lambda}\right)^2$

The second term on the lefthand side of equation B13 upon substitution of A16, A17, A18 becomes:

$$D\frac{\partial\theta}{\partial x'}\left[\frac{\partial z'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right] = \frac{D}{t^{1/2}}\frac{d\theta}{d\lambda}\left[\frac{\partial z'}{\partial\theta}\frac{\partial\theta}{\partial x'} - t\left(\frac{d\chi}{d\lambda}\right)^2\right]$$

$$= \frac{D}{t^{1/2}}\frac{d\theta}{d\lambda}\left[\frac{1}{t^{1/2}}\frac{d\theta}{d\lambda}\frac{\partial z'}{\partial\theta} - t\left(\frac{d\chi}{d\lambda}\right)^2\right]$$

$$= \frac{D}{t}\left(\frac{d\theta}{d\lambda}\right)^2\frac{\partial z'}{\partial\theta} - t^{1/2}D\frac{d\theta}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2$$

$$= \frac{P}{t}\frac{\partial z'}{\partial\theta} - t^{1/2}Q \qquad \text{(B14)}$$

where $Q = D\frac{d\theta}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2$

Similarly, the term on the righthand side of equation B13 is rearranged as follows:

$$\frac{\partial}{\partial c}\left[\theta D_s\frac{\partial c}{\partial x'}\left(\frac{\partial z'}{\partial x'} - \frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'}\right)\right] = \frac{\partial}{\partial c}\left[\frac{\theta D_s}{t^{1/2}}\frac{dc}{d\lambda}\left(\frac{\partial z'}{\partial c}\frac{\partial c}{\partial x'} - t\left(\frac{d\chi}{d\lambda}\right)^2\right)\right]$$

$$= \frac{\partial}{\partial c}\left[\frac{\theta D_s}{t^{1/2}}\frac{dc}{d\lambda}\left\{\frac{1}{t^{1/2}}\frac{dc}{d\lambda}\frac{\partial z'}{\partial c} - t\left(\frac{d\chi}{d\lambda}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial c}\left[\frac{\theta D_s}{t}\left(\frac{dc}{d\lambda}\right)^2\frac{\partial z'}{\partial c} - \theta D_s t^{1/2}\frac{dc}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2\right]$$

$$= \frac{\partial}{\partial c}\left[\frac{P_s(\theta)}{t}\frac{\partial z'}{\partial c} - t^{1/2}Q_s\right] \qquad \text{(B15)}$$

where $Q_s(\theta) = \theta D_s(\theta)\frac{dc}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^2$

Substitution of B14 and B15 into equation B13 yields

$$\theta\frac{\partial z'}{\partial t} - \left[\frac{P}{t}\frac{\partial z'}{\partial\theta} - t^{1/2}Q\right] = \frac{\partial}{\partial c}\left[\frac{P_s}{t}\frac{\partial z'}{\partial c} - t^{1/2}Q_s\right] \qquad \text{(B16)}$$

Let $\psi = \frac{z'}{t^{3/2}}$ $\qquad \frac{\partial z'}{\partial t} = \frac{3}{2}\,\psi t^{1/2}$

Also, $\frac{\partial z'}{\partial \theta} = \frac{\partial z'}{\partial \psi}\,\frac{\partial \psi}{\partial \theta} = t^{3/2}\,\frac{d\psi}{d\theta}$

and $\frac{\partial z'}{\partial c} = \frac{\partial z'}{\partial \psi}\,\frac{d\psi}{dc} = t^{3/2}\,\frac{d\psi}{dc}$

Equation B16 therefore becomes:

$$\frac{3}{2}\,\theta\psi t^{1/2} - [\frac{P}{t}\,t^{3/2}\,\frac{d\psi}{d\theta} - t^{1/2}\,Q] = \frac{\partial}{\partial c}\,[\frac{P_s}{t}\,t^{3/2}\,\frac{d\psi}{dc} - t^{1/2}\,Q_s]$$

Therefore,

$$\frac{3}{2}\,\theta\psi - P(\theta)\,\frac{d\psi}{d\theta} + Q(\theta) = \frac{d}{dc}\,[P_s(\theta)\,\frac{d\psi}{dc} - Q_s(\theta)\,] \qquad \text{(B17)}$$

Ordinary differential equation for ω:

This is started by subtracting equation B13 from B12, to obtain:

$$\theta\frac{\partial(z-z')}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\,[(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}) - (\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2)\,]$$

$$= \frac{\partial}{\partial c}\,[\theta D_s\,\frac{\partial c}{\partial x'}\{\,(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}) - (\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2)\,\}\,]$$

Let w = z-z'

$$\theta\frac{\partial w}{\partial t} - D\,\frac{\partial\theta}{\partial x'}\,[(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}) - \{\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2\,\}\,]$$

$$= \frac{\partial}{\partial c}\,[\theta D_s\,\frac{\partial c}{\partial x'}\,\{\,(\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'}) - (\frac{\partial y}{\partial x}\,\frac{\partial y'}{\partial x'} - (\frac{\partial y'}{\partial x'})^2)\,\}\,] \qquad \text{(B18)}$$

In equation B18,

$$\frac{\partial z}{\partial x} - \frac{\partial z'}{\partial x'} = \frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'}\frac{\partial y}{\partial x} \quad \text{(refer to equation A22)}$$

Also, from equation A24,

$$\frac{\partial y}{\partial x}\frac{\partial y'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2 = \frac{\partial y'}{\partial x'}\left[\frac{\partial z}{\partial x} - \frac{\partial y'}{\partial x'}\frac{\partial y}{\partial x}\right]$$

And so, substitution of equation A22 and A24 into B18 yields:

$$\theta\frac{\partial w}{\partial t} - D\frac{\partial \theta}{\partial x'}\left[\left(\frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'}\frac{\partial y}{\partial x}\right) - \frac{\partial y'}{\partial x'}\left(\frac{\partial z}{\partial x} - \frac{\partial y'}{\partial x'}\frac{\partial y}{\partial x}\right)\right]$$

$$= \frac{\partial}{\partial c}\left[\theta D_s\frac{\partial c}{\partial x'}\left\{\left(\frac{\partial w}{\partial x} - \frac{\partial z'}{\partial x'}\frac{\partial y}{\partial x}\right) - \frac{\partial y'}{\partial x'}\left(\frac{\partial z}{\partial x} - \frac{\partial y'}{\partial x'}\frac{\partial y}{\partial x}\right)\right\}\right] \qquad \text{(B19)}$$

Approximation 3:

Let $\frac{\partial w}{\partial x} = \frac{\partial w'}{\partial x'}$, $\frac{\partial y}{\partial x} = \frac{\partial y'}{\partial x'}$, $\frac{\partial z}{\partial x} = \frac{\partial z'}{\partial x'}$

Equation B19 becomes:

$$\theta\frac{\partial w'}{\partial t} - D\frac{\partial \theta}{\partial x'}\left[\left(\frac{\partial w'}{\partial x'} - \frac{\partial z'}{\partial x'}\frac{\partial y'}{\partial x'}\right) - \frac{\partial y'}{\partial x'}\left\{\frac{\partial z'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial c}\left[\theta D_s\frac{\partial c}{\partial x'}\left\{\left(\frac{\partial w'}{\partial x'} - \frac{\partial z'}{\partial x'}\frac{\partial y'}{\partial x'}\right) - \frac{\partial y'}{\partial x'}\left\{\frac{\partial z'}{\partial x'} - \left(\frac{\partial y'}{\partial x'}\right)^2\right\}\right\}\right] \qquad \text{(B20)}$$

Now, $x' = \lambda t^{1/2}$, $y' = \chi t$, $z' = \psi t^{3/2}$

Substitute A26, A27, A28 into B20 to obtain:

$$\theta\frac{\partial w'}{\partial t} - \frac{D}{t^{1/2}}\frac{d\theta}{d\lambda}\left[\frac{1}{t^{1/2}}\frac{\partial w'}{\partial\theta}\frac{\partial\theta}{\partial\lambda} - t\frac{d\psi}{d\lambda}t^{1/2}\frac{d\chi}{d\lambda} - t^{1/2}\frac{d\chi}{d\lambda}\left\{t\frac{d\psi}{d\lambda} - t\left(\frac{d\chi}{d\lambda}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial c}\left[\theta D_s\frac{1}{t^{1/2}}\frac{dc}{d\lambda}\left\{\frac{1}{t^{1/2}}\frac{\partial w'}{\partial c}\frac{dc}{d\lambda} - t\frac{d\psi}{d\lambda}t^{1/2}\frac{d\chi}{d\lambda} - t^{1/2}\frac{d\chi}{d\lambda}\left(t\frac{d\psi}{d\lambda} - t\left(\frac{d\chi}{d\lambda}\right)^2\right)\right\}\right]$$

Therefore,

$$\theta\frac{\partial w'}{\partial t} - \left\{\frac{D}{t}\left(\frac{d\theta}{d\lambda}\right)^2\frac{\partial w'}{\partial\theta} - 2Dt\frac{d\theta}{d\lambda}\frac{d\psi}{d\lambda}\frac{d\chi}{d\lambda} + Dt\frac{d\theta}{d\lambda}\left(\frac{d\chi}{d\lambda}\right)^3\right\}$$

$$= \frac{\partial}{\partial c}\left[\frac{\theta D_s}{t}\left(\frac{dc}{d\lambda}\right)^2\frac{\partial w'}{\partial c} - 2\theta D_s t\frac{dc}{d\lambda}\frac{d\psi}{d\lambda}\frac{d\chi}{d\lambda} + \theta D_s\frac{dc}{d\lambda}t\left(\frac{d\chi}{d\lambda}\right)^3\right]$$

$$\theta\frac{\partial w'}{\partial t} - \left[\frac{P}{t}\frac{\partial w'}{\partial\theta} - tD\frac{d\theta}{d\lambda}\frac{d\chi}{d\lambda}\left\{2\frac{d\psi}{d\lambda} - \left(\frac{d\chi}{d\lambda}\right)^2\right\}\right]$$

$$= \frac{\partial}{\partial c}\left[\frac{P_s}{t}\frac{\partial w'}{\partial c} - t\theta D_s\frac{dc}{d\lambda}\frac{d\chi}{d\lambda}\left\{2\frac{d\psi}{d\lambda} - \left(\frac{d\chi}{d\lambda}\right)^2\right\}\right] \qquad \text{(B21)}$$

Let $R = D\frac{d\theta}{d\lambda}\frac{d\chi}{d\lambda}\left[2\frac{d\psi}{d\lambda} - \left(\frac{d\chi}{d\lambda}\right)^2\right]$ and

$$R_s = \theta D_s\frac{dc}{d\lambda}\frac{d\chi}{d\lambda}\left[2\frac{d\psi}{d\lambda} - \left(\frac{d\chi}{d\lambda}\right)^2\right]$$

Equation B21 becomes:

$$\theta\frac{\partial w'}{\partial t} - \left(\frac{P}{t}\frac{\partial w'}{\partial\theta} - tR\right) = \frac{\partial}{\partial c}\left[\frac{P_s}{t}\frac{\partial w'}{\partial c} - tR_s\right] \qquad \text{(B22)}$$

Let $\omega = \frac{w'}{t^2}$, $\frac{\partial w'}{\partial t} = 2\omega t$

Also, $\frac{\partial w'}{\partial \theta} = \frac{\partial w'}{\partial \omega} \frac{\partial \omega}{\partial \theta} = t^2 \frac{d\omega}{d\theta}$

$$2\theta\omega t - \left(\frac{P}{t} t^2 \frac{d\omega}{d\theta} - tR\right) = \frac{d}{dc} \left[\frac{P_s}{t} t^2 \frac{d\omega}{dc} - tR_s \right]$$

Therefore,

$$2\theta\omega - \left(P(\theta) \frac{d\omega}{d\theta} - R(\theta) \right) = \frac{d}{dc} \left[P_s(\theta) \frac{d\omega}{dc} - R_s(\theta) \right] \qquad \text{(B23)}$$

APPENDIX C1

Description of Computer Program for Calculating Hydraulic Conductivity as a Function of Water Content

The actual computer program for calculating K(θ) is given in figures C1 and C2. In figure C1, values for D and corresponding water contents $\theta (= \frac{\theta - \theta_n}{\theta_o - \theta_n})$ and also soil water suction SWS and corresponding θ are provided in FUNCTION DIFF and FUNCTION MRC, respectively. By renaming Time = SWS, derivatives are performed with respect to SWS. In the DYNAMIC section of figure C1, a non-linear interpolation (Lagrange quadratic interpolation) is used to determine θ and D through the statements:

```
CTHETA = NLFGEN(MRC,SWS)
TDIFF  = NLFGEN(DIFF,CTHETA)
```

The derivative dθ/dh and hydraulic conductivity K are calculated using the statements:

```
DMRC   = DERIV(MRCO,CTHETA)
K      = -(THETAD-THETAN)*TDIFF*DMRC
```

Alternatively, the hydraulic conductivity may be calculated for various water contents by using the short program given in figure C2 in which FUNCTION TBTHLA and FUNCTION SWS are tables of values of water

FIGURE C1

Computer listing for calculating hydraulic conductivity as a function of water content.

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

           TITLE CALCULATION OF HYDRAULIC CONDUCTIVITY (BROOKSTON CLAY)
           *     UNITS
           *     M=METERS
           *     S=SECONDS
           *     KG=KILOGRAMS
           *     GLOSSARY OF SYMBOLS
           *     SWS=SOIL WATER SUCTION
           *     DIFF=TABLE OF SOIL WATER DIFFUSIVITY AND CORRESPONDING WATER
           *     CONTENT VALUES
           *     MRC=TABLE OF SOIL WATER SUCTION AND CORRESPONDING WATER
           *     CONTENT VALUES
           *     DMRC=DERIVATIVE OF WATER CONTENT WITH RESPECT TO SOIL WATER
           *     SUCTION
           *     K=HYDRAULIC CONDUCTIVITY
           *     TDIFF=INTERPOLATED SOIL WATER DIFFUSIVITY VERSUS SOIL WATER
           *     SUCTION
           *     CTHETA=INTERPOLATED WATER CONTENT VERSUS SOIL WATER SUCTION
             RENAME TIME=SWS
           INITIAL
                  INCON THETAN=.12,THETAO=.53,MRCO=-.24417
                  FUNCTION DIFF=(0.0,1.2E-08),(.06,1.6E-08),(.1,1.9E-08),...
                  (.14,2.3E-08),(.2,3.1E-08),(.3,5.2E-08),(.36,7.2E-08),...
                  (.4,8.9E-08),(.44,1.1E-07),(.48,1.4E-07),(.5,1.55E-07),...
                  (.56,2.25E-07),(.6,2.9E-07),(.64,3.8E-07),(.68,5.0E-07),...
                  (.7,5.8E-07),(.74,8.0E-07),(.78,1.1E-06),(.8,1.3E-06),...
                  (.84,2.0E-06),(.88,3.2E-06),(.9,4.2E-06),(.92,5.8E-06),...
                  (.94,8.2E-06),(.96,1.3E-05),(.98,2.5E-05),(1.0,4.8E-05)
                  FUNCTION MRC=(0.0,1.0),(.05,.9878),(.1,.9756),(.15,.9512),...
                  (.2,.9146),(.25,.8659),(.3,.8293),(.35,.7805),(.4,.7317),...
                  (.45,.6829),(.5,.6463),(.55,.6098),(.605,.5854),(.655,.561),...
                  (.75,.5244),(.85,.4878),(.9,.4756),(.95,.4634),(1.0,.4512),...
                  (1.075,.439),(1.15,.4268),(1.2,.4146)
           DYNAMIC
                  CTHETA=NLFGEN(MRC,SWS)
                  TDIFF=NLFGEN(DIFF,CTHETA)
                  DMRC=DERIV(MRCO,CTHETA)
                  K=-(THETAO-THETAN)*TDIFF*DMRC
                  THLA=CTHETA*(THETAO-THETAN)+THETAN
           TERMINAL
                  PRINT DMRC,CTHETA,THLA,TDIFF,K
                  TIMER FINTIM=1.2,PRDEL=2.4E-02
           END
           STOP

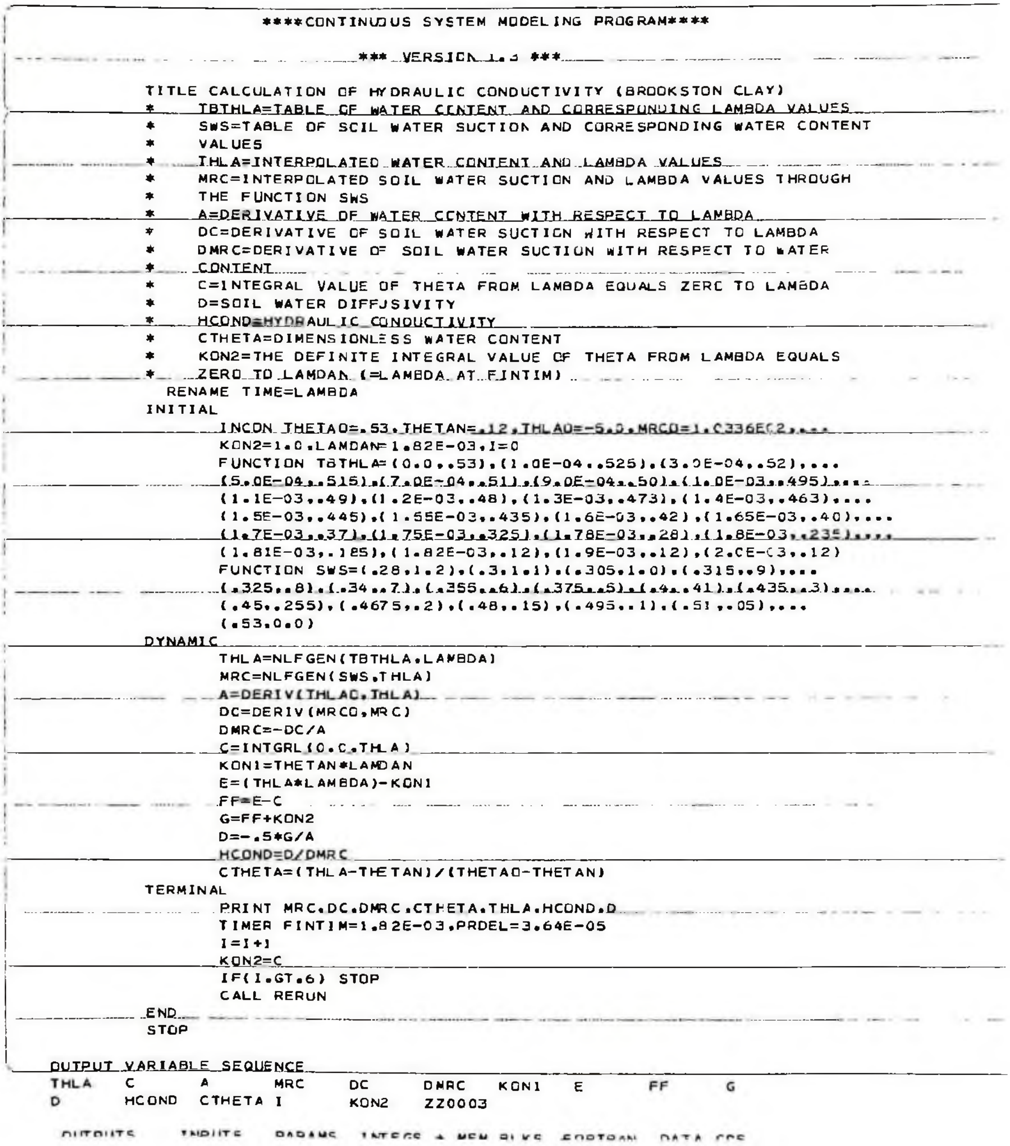
    OUTPUT VARIABLE SEQUENCE
    CTHETA DMRC    TDIFF   K       THLA

     OUTPUTS      INPUTS     PARAMS    INTEGS + MEM BLKS   FORTRAN   DATA CDS
      9(500)     33(1400)     7(400)     0+   0=  0(300)     6(600)       17

           ENDJOB
```

FIGURE C2

Alternate computer program using λ as the variable time, for calculating hydraulic conductivity as a function of water content.



```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                             *** VERSION 1.3 ***

       TITLE CALCULATION OF HYDRAULIC CONDUCTIVITY (BROOKSTON CLAY)
       *     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
       *     SWS=TABLE OF SOIL WATER SUCTION AND CORRESPONDING WATER CONTENT
       *     VALUES
       *     THLA=INTERPOLATED WATER CONTENT AND LAMBDA VALUES
       *     MRC=INTERPOLATED SOIL WATER SUCTION AND LAMBDA VALUES THROUGH
       *     THE FUNCTION SWS
       *     A=DERIVATIVE OF WATER CONTENT WITH RESPECT TO LAMBDA
       *     DC=DERIVATIVE OF SOIL WATER SUCTION WITH RESPECT TO LAMBDA
       *     DMRC=DERIVATIVE OF SOIL WATER SUCTION WITH RESPECT TO WATER
       *     CONTENT
       *     C=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO LAMBDA
       *     D=SOIL WATER DIFFUSIVITY
       *     HCOND=HYDRAULIC CONDUCTIVITY
       *     CTHETA=DIMENSIONLESS WATER CONTENT
       *     KON2=THE DEFINITE INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS
       *     ZERO TO LAMDAN (=LAMBDA AT FINTIM)
         RENAME TIME=LAMBDA
       INITIAL
                INCON THETAO=.53,THETAN=.12,THLAO=-5.0,MRCO=1.0336E02,...
                KON2=1.0,LAMDAN=1.82E-03,I=0
                FUNCTION TBTHLA=(0.0,.53),(1.0E-04,.525),(3.0E-04,.52),...
                (5.0E-04,.515),(7.0E-04,.51),(9.0E-04,.50),(1.0E-03,.495),...
                (1.1E-03,.49),(1.2E-03,.48),(1.3E-03,.473),(1.4E-03,.463),...
                (1.5E-03,.445),(1.55E-03,.435),(1.6E-03,.42),(1.65E-03,.40),...
                (1.7E-03,.37),(1.75E-03,.325),(1.78E-03,.28),(1.8E-03,.235),...
                (1.81E-03,.185),(1.82E-03,.12),(1.9E-03,.12),(2.0E-03,.12)
                FUNCTION SWS=(.28,1.2),(.3,1.1),(.305,1.0),(.315,.9),...
                (.325,.8),(.34,.7),(.355,.6),(.375,.5),(.4,.41),(.435,.3),...
                (.45,.255),(.4675,.2),(.48,.15),(.495,.1),(.51,.05),...
                (.53,0.0)
       DYNAMIC
                THLA=NLFGEN(TBTHLA,LAMBDA)
                MRC=NLFGEN(SWS,THLA)
                A=DERIV(THLAO,THLA)
                DC=DERIV(MRCO,MRC)
                DMRC=-DC/A
                C=INTGRL(0.C,THLA)
                KON1=THETAN*LAMDAN
                E=(THLA*LAMBDA)-KON1
                FF=E-C
                G=FF+KON2
                D=-.5*G/A
                HCOND=D/DMRC
                CTHETA=(THLA-THETAN)/(THETAO-THETAN)
       TERMINAL
                PRINT MRC,DC,DMRC,CTHETA,THLA,HCOND,D
                TIMER FINTIM=1.82E-03,PRDEL=3.64E-05
                I=I+1
                KON2=C
                IF(I.GT.6) STOP
                CALL RERUN
       END
       STOP

  OUTPUT VARIABLE SEQUENCE
  THLA     C        A        MRC      DC       DMRC     KON1     E        FF       G
  D        HCOND    CTHETA   I        KON2     ZZ0003

   OUTPUTS     INPUTS     PARAMS   INTEGS + MEM BLKS   FORTRAN   DATA CDS
```

content θ versus lambda ($\lambda = xt^{-1/2}$) and soil matric suction versus water content, respectively. Time in this program is renamed lambda and soil water diffusivity D calculated (see description in Section 4.9.1). Interpolated values for soil matric suction SWS and lambda is provided through the statement

```
MRC    = NLFGEN(SWS,THLA)
```

The derivatives, $d\theta/d\lambda$ and $dh/d\lambda$ are calculated respectively using the statements

```
A      = DERIV(THLAO,THLA)
DC     = DERIV(MRCO,MRC)
```

The derivative $dh/d\theta$ $(= \frac{dh}{d\lambda} \cdot \frac{d\lambda}{d\theta})$ is calculated using the statement:

```
DMRC   = -DC/A
```

The hydraulic conductivity K is then calculated through the statement:

```
HCOND = D/DMRC
```

Values of $K(\theta)$ for low moisture contents were obtained by extrapolation of the $K(\theta)$ curve.

APPENDIX C

Algorithm for the simulation of $\theta(\lambda)$ from calculated $D(\lambda)$ values

Assuming the objective is to simulate $\theta(\lambda)$ relationship in fig. 1c (curve c), RVELO(=D $d\theta/d\lambda$ at $\lambda=0$) is guessed. RVELAO is thus obtained through the multiplicative factor 1.0001. Using equations 4.28 through to 4.33, RVELO and RVELAO generate THETAO and THETAA respectively. The difference between these two generated $\theta(\lambda)$ functions, designated DTHETA, is then calculated, followed by the calculation of the slope which is done using the usual mathematical equation for a slope as follows:

The slope m, of the relationship between THETA2, THETAA and their respective RVELO and RVELAO (fig. 2c) is given by the equation

$$m = \frac{y_2 - y_1}{x_2 - x_1} = \frac{\text{THETAA} - \text{THETA2}}{\text{RVELAO} - \text{RVELO}} \qquad \text{(C1)}$$

But RVELAO-RVELO = RVELO x 1.0001 - RVELO

= RVELO(1.0001 - 1.0)

= 0.0001 RVELO

Therefore,

$$\text{SLOPE} = \text{DTHETA}/(.0001 \times \text{RVELO}) \qquad \text{(C2)}$$

The correction factor, DRVEL, required for the calculation of a 'new' RVELO, is the difference between the FINTIM value of the simulated moisture content and the initial moisture content θ_n, divided by the slope:

Figure 1c: Schematic representation of $\theta(\lambda)$ function with two θ curves generated by RVELO and RVELAO.

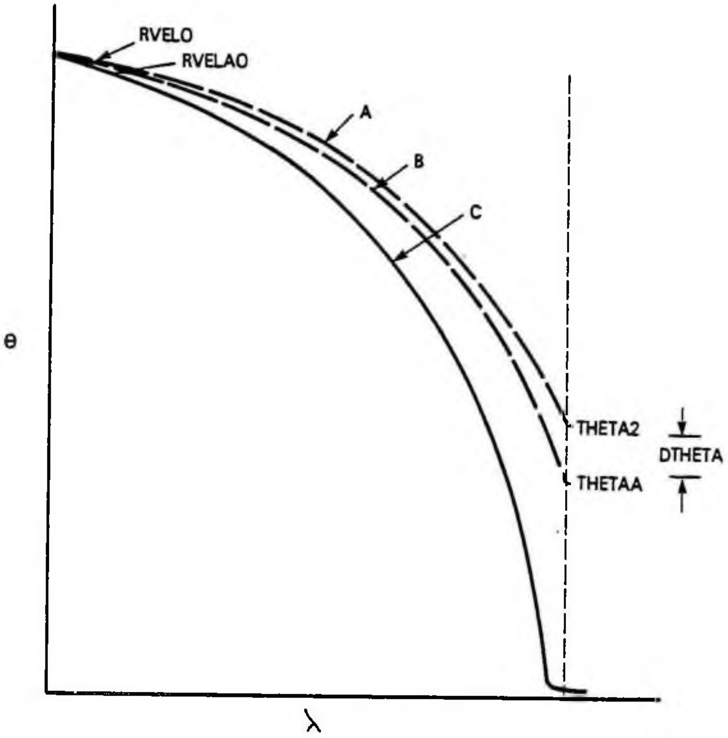


Figure 1c.

Figure 2c: Schematic plot of THETA2 and THETAA at $\lambda = 0$ versus their corresponding RVELO and REVELAO.

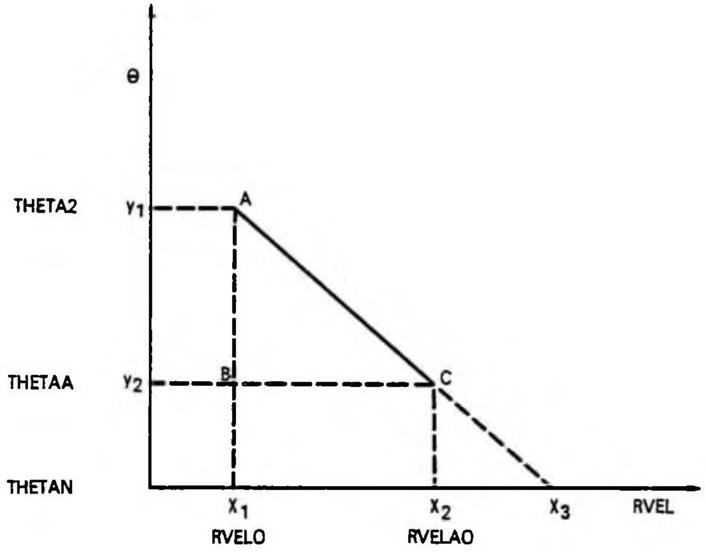


Figure 2c.

DRVEL = (THETA2-THETAN)/SLOPE

This relationship for DRVEL is obtained from the consideration of fig. 2c as follows:

By the *theorem of similar triangles, ABC and Ax_1x_3 are congruent. Therefore,

$$\frac{\text{RVELAO} - \text{RVELO}}{\text{THETAA} - \text{THETA2}} = \frac{x_3 - x_1}{\text{THETA2} - \text{THETAN}}$$

From equation C1

$$\frac{\text{RVELAO} - \text{RVELO}}{\text{THETAA} - \text{THETA2}} = \frac{1}{\text{SLOPE}}$$

Therefore,

$$\text{DRVEL} = x_3 - x_1 = (\text{THETA2} - \text{THETAN})/\text{SLOPE}$$

The 'new' RVELO to be used for the next iteration is the old RVELO minus DRVEL. In CSMP, this is written as:

RVELO = RVELO - DRVEL

---

* Theorem states that if corresponding angles of two triangles are equal, then their corresponding sides are proportional.

The specification in the algorithm (fig. 4.5) that iteration should stop when simulated THETA2 has converged sufficiently so that the absolute value of the difference between FINTIM value of THETA2 and θ_n (THETAN) is less than 0.00001, ensures that the simulation stops at that accuracy. Failure to converge, the specification on the counters, that is, IF(J.GT.10)STOP and IF(I.GT.6)STOP will terminate the simulation.

APPENDIX D

Algorithm for the simulation of $c(\lambda)$ for the calculated $D_s(\lambda)$ values

The development of the algorithm for the simulation of $c(\lambda)$ is similar to that for $\theta(\lambda)$ given in Appendix A. The main difference is that VELCO (equivalent to RVELO in Appendix C) is equal to $\theta D_s \frac{dc}{d\lambda}$ at $\lambda=0$.

Here, the objective is to simulate $c(\lambda)$ relationship in fig. 1D (curve f). VELCO is guessed. This guess yields VELCAO because of the multiplying factor 1.00001. Equations 4.54 through to 4.58b are then used to simulate SEE2 and its half pair SEEA, respectively. DSEE which is the difference between these two generated $c(\lambda)$ functions is calculated. Then the slope which from equations similar to C1 and C2 is equal to DSEE/(.00001 x VELCO) is computed. The correction factor, DVELC, is then obtained from the difference between the simulated c at FINTIM and the initial concentration c_n (specified in the PARAMETER section) divided by the slope. The 'new' VELCO to be used for the next iteration is obtained by subtracting the correction factor from the 'old' VELCO.

When simulated concentration values converge sufficiently the simulation is terminated due to the specification for simulation to stop when the absolute value of the difference between SEE2 and SEEN is less than .00005. Otherwise the stop specifications on the counters I and J will terminate simulation.

Figure 1d: Schematic representation of $c(\lambda)$ function depicting the two c curves generated by VELCO and VELCAO.

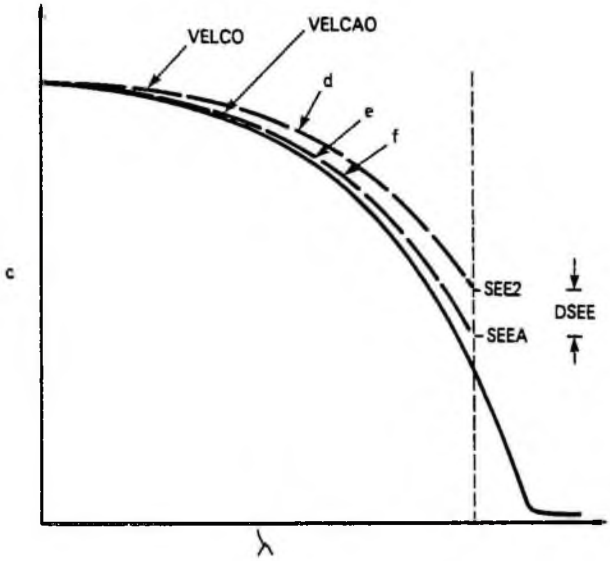


Figure 1d.

APPENDIX E

CSMP listing for calculating soil water diffusivity D and simulation of $\theta(\lambda)$ for Akuse clay

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

       TITLE CALCULATION OF SOIL MOISTURE DIFFUSIVITY AND SIMULATION OF
       TITLE WATER CONTENT AS A FUNCTION OF LAMBDA  (AKUSE CLAY)
       *     UNITS
       *     KG=KILOGRAMS
       *     M=METERS
       *     S=SECONDS
       *     GLOSSARY OF SYMBOLS
       *     DTHLAO=DERIVATIVE OF THE THETA-LAMBDA FUNCTION AT LAMBDA EQUALS
       *     ZERO
       *     THETAO=WATER CONTENT AT LAMBDA EQUALS ZERO
       *     LAMDAN=LAMBDA AT INFINITY (=FINTIM)
       *     THETAN=INITIAL WATER CONTENT
       *     THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
       *     RVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY AND THE DERIVATIVE
       *     OF THE THETA-LAMBDA FUNCTION
       *     RVELO=RVEL AT LAMBDA EQUALS ZERO
       *     D=SOIL WATER DIFFUSIVITY
       *     RDIV=DERIVATIVE OF RVEL WITH RESPECT TO LAMBDA
       *     RVELAO=RVELO MULTIPLIED BY 1.0001
       *     RVELA=HALF PAIR OF RVEL THROUGH THE FACTOR 1.0001 IN RVELAO
       *     RDIVA=HALF PAIR OF RDIV THROUGH THE FACTOR 1.0001
       *     THETA2=SIMULATED WATER CONTENT
       *     THETAA=HALF PAIR OF THETA2 THROUGH THE FACTOR 1.0001
       *     DRVEL=CORRECTION FACTOR
       *     DTHETA=DIFFERENCE BETWEEN THETA2 AND THETAA
       *     SLOPE=RATIO OF THE DIFFERENCE BETWEEN THETAA AND THETA2 TO THE
       *     DIFFERENCE BETWEEN RVELAO AND RVELO
       *     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
         RENAME TIME=LAMBDA
       INITIAL
             PARAMETER DTHLAO=-1.0E01,THETAO=.526,LAMDAN=4.56E-03,...
             THETAN=.10,KON2=1.0,RVELO=-.8746528E-03,I=0,J=0,DEL=.0001
             RVELAO=RVELO*(1.0+DEL)
             FUNCTION TBTHLA=(0.0,.526),(1.0E-04,.525),(2.0E-04,.524),....
             (6.0E-4,.52),(1.2E-3,.515),(1.85E-3,.51),(2.2E-3,.505),....
             (2.4E-3,.504),(2.5E-3,.503),(2.6E-3,.50),(3.0E-3,.495),...
             (3.2E-3,.4875),(3.4E-3,.480),(3.5E-3,.475),(3.6E-3,.470),...
             (3.7E-3,.464),(3.8E-3,.455),(3.9E-3,.4475),(4.0E-3,.435),....
             (4.1E-3,.420),(4.2E-3,.40),(4.3E-3,.370),(4.40E-3,.33),....
             (4.46E-3,.295),(4.50E-3,.250),(4.56E-3,.10),(5.0E-3,.10)
       DYNAMIC
             THLA=NLFGEN(TBTHLA,LAMBDA)
             DTHLA=DERIV(DTHLAO,THLA)
             THETA1=INTGRL(THETAO,DTHLA)
             C=INTGRL(0.0,THLA)
             KON1=THETAN*LAMDAN
             E=(THLA*LAMBDA)-KON1
             FF=E-C
             G=FF+KON2
             D=-.5*G/DTHLA
             NOSORT
             IF(J.LE.2) GO TO 10
             SORT
             RVEL=INTGRL(RVELO,RDIV)
             RVELA=INTGRL(RVELAO,RDIVA)
             RDIV=-LAMBDA*RVEL*.5/D
             RDIVA=-LAMBDA*RVELA*.5/D
             THETA2=INTGRL(THETAO,RVEL/D)
             THETAA=INTGRL(THETAO,RVELA/D)
             NOSORT
         10  CONTINUE
```

```
         TERMINAL
                 TIMER FINTIM=4.56E-03,PRDEL=9.12E-05
                 PRINT G,THETAA,D,THETA1,THLA,THETA2
                 IF(J.GE.3) GO TO 15
                 J=J+1
                 KON2=0
                 GO TO 20
          15     I=I+1
                 IF(ABS(THETA2-THETAN).LT..00001) STOP
                 DTHETA=THETAA-THETA2
                 SLOPE=DTHETA/DEL/RVELO
                 DRVEL=(THETA2-THETAN)/SLOPE
                 RVELO=RVELO-DRVEL
                 RVELAO=RVELO*(1.0+DEL)
                 WRITE(6,100) THETAA,D,THLA,THETA1,THETA2
         100     FORMAT(///' THETAA,D,THLA,THETA1,THETA2=',5E15.6)
                 WRITE (6,101) RVELO,RVELAO
         101     FORMAT(//' CALL RERUN WITH RVELO,RVELAO=',2E20.7)
          20     IF(J.GT.10) STOP
                 IF(I.GT.6) STOP
                 CALL RERUN
         END
         STOP

OUTPUT VARIABLE SEQUENCE
RVELAO THLA    DTHLA   THETA1 C       KON1    E       FF      G       D
ZZ0004 RDIV    RVEL    RDIVA  RVELA   ZZ0008  THETA2  ZZ0010  THETAA  ZZ0011
ZZ0012 J       KON2    I      DTHETA  SLOPE   DRVEL   RVELO   RVELAO

 OUTPUTS    INPUTS    PARAMS   INTEGS + MEM BLKS   FORTRAN   DATA CDS
 33(600)   71(1400)   12(400)    6+  0=  6(300)    39(600)      14


         ENDJOB
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APPENDIX F

CSMP listing for calculating dispersion coefficient D_s for Cl^- and simulation of $c(\lambda)$ using (i) analytical solution and (ii) computer solution (Akuse clay)

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

TITLE DISPERSION COEFFICIENT AND SIMULATION OF CONC. (AKUSE CLAY)
*     UNITS
*     KEQ=KILO-EQUIVALENTS
*     M=METERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     DTHLAO=DERIVATIVE OF THETA-LAMBDA FUNCTION AT LAMBDA
*     EQUALS ZERO
*     DTHLA=DERIVATIVE OF THETA -LAMBDA FUNCTION
*     THETAO=VOLUMETRIC WATER CONTENT AT LAMBDA EQUALS ZERO
*     LAMDAN=LAMBDA AT INFINITY (=FINTIM)
*     THETAN=INITIAL WATER CONTENT
*     THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
*     VELC=THE PRODUCT OF WATER CONTENT, DISPERSION COEFFICIENT
*     AND THE DERIVATIVE OF THE CONTRATION-LAMBDA FUNCTION
*     VELCO=VELC AT LAMBDA EQUALS ZERO
*     VELCAC=VELCO MULTIPLIED BY 1.00001
*     SEEO=CONCENTRATION OF CHLORIDE IN SOLUTION AT LAMBDA EQUALS
*     ZERO
*     SEEN=INITIAL CONCENTRATION OF CHLORIDE IN MOIST SOIL
*     DSEELA=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION WITH RESPECT
*     TO LAMBDA
*     DSELAO=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION AT LAMBDA
*     EQUALS ZERO
*     SEELA=INTERPOLATED CURVE FOR CONCENTRATION-LAMBDA FUNCTION
*     LATHH=THE G-FUNCTION DEFINED IN EQUATION 4.34
*     TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
*     TBSELA=TABLE OF CONCENTRATION OF CHLORIDE IN SOLUTION AND
*     CORRESPONDING LAMBDA VALUES
*     D=SOIL WATER DIFFUSIVITY
*     DIV=DERIVATIVE OF VELC WITH RESPECT TO LAMBDA
*     SEE2=SIMULATED CONCENTRATION OF CHLORIDE IN SOLUTION
*     SEE1=CONCENTRATION OF CHLORIDE CALCULATED USING THE ANALYTICAL
*     SOLUTION
*     SEEA=HALF PAIR OF SEE2 THROUGH THE FACTOR 1.00001
*     DVELC=CORRECTION FACTOR
*     SLOPE=RATIO OF THE DIFFERENCE BETWEEN SEEA AND SEE2 TO THE
*     DIFFERENCE BETWEEN VELCAC AND VELCO
*     DSEE=DIFFERENCE BETWEEN SEE2 AND SEEA AT FINTIM
   RENAME TIME=LAMBDA
INITIAL
         INCON THETAN=.10,LAMCAN=4.56E-03,KON2=1.0,KON3=1.0,KON4=1.0
         PARAMETER DSELAO=-1.0,SEEO=.92,DTHLAO=-1.0E01,THETAO=.520
         CONSTANT SEEN=.00006,I=0,J=0,...
         VELCO=-.717991SE-04,DEL=.00001
         VELCAO=VELCO*(1.0+DEL)
         FUNCTION TBTHLA=(0.0,.526),(1.0E-04,.525),(2.0E-04,.524),...
         (6.0E-4,.52),(1.2E-3,.515),(1.8E-3,.51),(2.2E-3,.505)....
         (2.4E-3,.504),(2.5E-3,.503),(2.8E-3,.50),(3.0E-3,.495),...
         (3.2E-3,.4875),(3.4E-3,.480),(3.5E-3,.470),(3.6E-3,.47)),...
         (3.7E-3,.464),(3.8E-3,.455),(3.9E-3,.4475),(4.0E-3,.435),...
         (4.1E-3,.420),(4.2E-3,.40),(4.3E-3,.370),(4.40E-3,.33),...
         (4.46E-3,.295),(4.50E-3,.250),(4.56E-3,.10),(5.0E-3,.10)
         FUNCTION TBSELA=(0.0,.92),(1.0E-04,.9199),(2.0E-04,.9198),...
         (3.0E-04,.9197),(4.0E-04,.9196),(5.0E-04,.9195),...
         (6.0E-04,.9194),(7.0E-04,.9193),(8.0E-04,.9192),...
         (9.0E-04,.9191),(1.0E-03,.919),(1.1E-03,.9189),...
         (1.2E-03,.9188),(1.3E-03,.9187),(1.4E-03,.9186),...
         (1.5E-03,.9185),(1.6E-03,.9184),(1.7E-03,.9183),...
         (1.8E-03,.9182),(1.9E-03,.9181),(2.0E-03,.918),...
```

```
         (2.1E-03,.9179),(2.2E-03,.91)....
         (2.4E-03,.905),(2.6E-03,.90),(2.7E-03,.89),(2.8E-03,.88)....
         (2.9E-03,.87),(3.0E-03,.86),(3.1E-03,.84),(3.2E-03,.82)....
         (3.3E-03,.80),(3.4E-03,.77),(3.5E-03,.735),(3.6E-03,.695)....
         (3.7E-03,.645),(3.8E-03,.585),(3.9E-03,.[illegible]),(4.0E-3,.38)....
         (4.1E-03,.20),(4.12E-03,.17),(4.14E-03,.14),(4.16E-3,.12)....
         (4.18E-03,.09),(4.2E-03,.075),(4.22E-03,.06),(4.24E-3,.04)....
         (4.26E-03,.03),(4.28E-03,.02),(4.3E-03,.015),(4.34E-03,.01)....
         (4.36E-03,.008),(4.38E-03,.006),(4.4E-03,.004)....
         (4.42E-03,.002),(4.44E-03,.0009),(4.46E-03,.0007)....
         (4.4688E-03,.0006),(4.48E-03,.0005),(4.5E-03,.0003)....
         (4.52E-03,.0001),(4.54E-03,.00008),(4.56E-03,.00006)....
         (4.57E-03,.00005),(4.58E-03,.00004)
 DYNAMIC
         THLA=NLFGEN(TBTHLA,LAMBDA)
         SEELA=NLFGEN(TBSELA,LAMBDA)
         CTHETA=(THLA-THETAN)/(THETAD-THETAN)
         CSEE=(SEELA-SEEN)/(SEEO-SEEN)
         DTHLA=DERIV(DTHLAO,THLA)
         DSEELA=DERIV(DSELAO,SEELA)
         C=INTGRL(0.0,THLA)
         KON1=THETAN*LAMDAN
         E=(THLA*LAMBDA)-KON1
         FF=E-C
         G=FF+KON2
         D=-.5*G/DTHLA
         LATHH=(THLA*LAMBDA)+(2.0*D*DTHLA)
         GS=DSEELA*LATHH
         HS=INTGRL(0.0,GS)
         HS1=KON3-HS
         HS2=.5*HS1
         THDS=HS2/DSEELA
         DS=THDS/THLA
         NOSORT
         IF(I.LT.3) GO TO 10
         IF(THDS.EQ.0.0) GO TO 10
         SORT
         AH=LATHH/THDS
         BH=INTGRL(0.0,AH)
         CH=EXP(-.5*BH)
         MH=INTGRL(0.0,CH/THDS)
         RMH=MH/KON4
         SEE1=RMH*(SEEN-SEEO)+SEEO
         VELC=INTGRL(VELCO,RDIV)
         VELCA=INTGRL(VELCAO,RDIVA)
         RDIV=-(LATHH*VELC)/(2.0*THDS)
         RDIVA=-(LATHH*VELCA)/(2.0*THDS)
         SEE2=INTGRL(SEEO,VELC/THDS)
         SEEA=INTGRL(SEEO,VELCA/THDS)
         NOSORT
   10    CONTINUE
 TERMINAL
         METHOD SIMP
         PRINT THLA,D,THDS,DS,AH,SEELA,SEE1,SEE2
         TIMER FINTIM=4.56E-03,DELT=5.0E-06,PRDEL=9.12E-05
         I=I+1
         KON2=C
         KON3=HS
         IF(I.LT.4) GO TO 20
         KON4=MH
         IF(ABS(SEE2-SEEN).LT..000001) STOP
         DSEE=SEEA-SEE2
         SLOPE=DSEE/DEL/VELCO
         DVELC=(SEE2-SEEN)/SLOPE
         VELCO=VELCO-DVELC
         VELCAO=VELCO*(1.0+DEL)
```

```
                WRITE(6,100) KON2,KON3,KON4
          100   FORMAT(///' KON2,KON3,KON4=',3E15.6)
                WRITE(6,101) DSEE,SLOPE,DVELC
          101   FORMAT(///' DSEE,SLOPE,DVELC=',3E15.6)
                WRITE(6,103) VELCC,VELCAC
          103   FORMAT(//' CALL RERUN WITH VELCC,VELCAU=',2E20.7)
          20    IF(I.GT.10) STOP
                CALL RERUN
         END
         STOP

OUTPUT VARIABLE SEQUENCE
VELCAO THLA    C       DTHLA   KON1    E       FF      G       J       LATHH
SEELA  DSEELA  GS      HS      CTHETA  CSEE    HS1     HS2     THDS    DS
ZZ0005 AH      BH      CH      ZZ0010  MH      RDIV    VELC    RDIVA   VELCA
ZZ0014 SEE2    ZZ0016  SEEA    RMH     SEE1    ZZ0017  I       KON2    KON3
ZZ0018 KON4    DSEE    SLOPE   DVELC   VELCC   VELCAC

 OUTPUTS     INPUTS     PARAMS    INTEGS + MEM BLKS    FORTRAN    DATA CDS
 51(500)   110(1400)   19(400)    84   3=   8(300)     58(600)      3

         ENDJOB
```

APPENDIX G

CSMP listing for calculating dispersion coefficient D_s for K^+ and simulation of $c(\lambda)$ from the computed $D_s(\lambda)$ values for Akuse clay

```
                    ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

TITLE DS FOR POTASSIUM AND SIMULATION OF CONCENTRATION (AKUSE CLAY)
*       UNITS
*       KEQ=KILO-EQUIVALENTS
*       KG=KILOGRAMS
*       M=METERS
*       S=SECONDS
*       GLOSSARY OF SYMBOLS
*       LAMDAN=LAMBDA AT INFINITY (=FINTIM)
*       THLA=INTERPOLATED CURVE FOR THETA-LAMBDA FUNCTION
*       VELK=PRODUCT OF THE WATER CONTENT ,DISPERSION COEFFICIENT AND
*       THE DERIVATIVE OF THE CENTRATION -LAMBDA FUNCTION
*       VELKO=VELK AT LAMBDA EQUALS ZERO
*       VELKA=HALF PAIR OF VELK THROUGH THE FACTOR 1.0001
*       VELKAO=VELKO MULTIPLIED BY 1.0001
*       SEEO=CONCENTRATION OF POTASSIUM IN SOLUTION AT LAMBDA EQUALS
*       ZERO
*       SEEN=INITIAL CONCENTRATION OF POTASSIUM IN SOLUTION IN THE
*       MOIST SOIL
*       DSELAO=DERIVATIVE OF CONCENTRATION-LAMBDA FUNCTION AT LAMBDA
*       EQUALS ZERO
*       SEELA=INTERPOLATED CURVE FOR CONCENTRATION-LAMBDA FUNCTION
*       TBTHLA=TABLE OF WATER CONTENT AND CORRESPONDING LAMBDA VALUES
*       TBSELA=TABLE OF CONCENTRATION OF POTASSIUM IN SOLUTION AND
*       CORRESPONDING LAMBDA VALUES
*       ADSISO=ADSORPTION ISOTHERM
*       SS=INTERPOLATED CURVE FOR KILO-EQUIVALENT OF POTASSIUM
*       ADSORBED PER KILOGRAM SOIL. INTERPOLATION IS WITH RESPECT
*       TO LAMBDA THROUGH THE ADSORPTION ISOTHERM
*       DSSO=DERIVATIVE OF SS AS AFUNCTION OF LAMBDA AT LAMBDA EQUALS
*       ZERO
*       DSEELA=DERIVATIVE OF CONCENTRATION -LAMBDA RELATION
*       DSS=DERIVATIVE OF SS WITH RESPECT TO LAMBDA
*       D=SOIL WATER DIFFUSIVITY
*       DTHLA=DERIVATIVE OF WATER CONTENT WITH RESPECT TO LAMBDA
*       C=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO LAMBDA
*       KON2=DEFINITE INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO
*       LAMDAN (=LAMBDA AT FINTIM)
*       DS=DISPERSION COEFFICIENT
*       DIV=DERIVATIVE OF VELK WITH RESPECT TO LAMBDA
*       DIVA=HALF PAIR OF DIV THROUGH THE FACTOR 1.0001
*       SEE1=SIMULATED CONCENTRATION OF POTASSIUM IN SOLUTION
*       SEEA=HALF PAIR OF SEE1 THROUGH THE FACTOR 1.0001
*       DSEE=DIFFERENCE BETWEEN SEEA AND SEE1 AT FINTIM
*      SSLOPE=RATIO OF DSEE TO THE DIFFERENCE BETWEEN VELKAO AND VELKO
*       DRVEL=CORRECTION FACTOR
    RENAME TIME=LAMBDA
INITIAL
          INCON VELKO=-.5339585E-04,FLAG=0,SEEN=0.0,THETAN=.10,...
          BO=.24E-03,LAMDAN=4.56E-03,DEL=.0001,SEEO=1.05
          PARAMETER DSELAO=-2.51E-01,DSSO=-2.3E-05,RHO=1.03E03
          CONSTANT KON2=1.0,KON3=1.0,I=0,J=0,DTHLAO=-1.0E01
          VELKAO=VELKO*(1.0+DEL)
          FUNCTION TBTHLA=(0.0,.526),(1.0E-04,.525),(2.0E-04,.524),...
          (6.0E-4,.52),(1.2E-3,.515),(1.8E-3,.51),(2.2E-3,.505),...
          (2.4E-3,.504),(2.5E-3,.503),(2.6E-3,.50),(3.0E-3,.495),...
          (3.2E-3,.4875),(3.4E-3,.480),(3.5E-3,.475),(3.6E-3,.470),...
          (3.7E-3,.464),(3.8E-3,.455),(3.9E-3,.4475),(4.0E-3,.435),...
          (4.1E-3,.420),(4.2E-3,.40),(4.3E-3,.370),(4.40E-3,.33),...
          (4.46E-3,.295),(4.50E-3,.250),(4.56E-3,.10),(5.0E-3,.10)
```

```
          FUNCTION TBSELA=(0.0,1.09),(4.0E-04,1.0899),(8.0E-04,1.0898)....
          (1.2E-3,1.0897),(1.4E-3,1.0896),(1.68E-3,1.08)....
          (1.80E-3,1.06)....
          (1.9E-3,1.03),(2.0E-3,.99),(2.1E-3,.93),(2.14E-3,.90)....
          (2.2E-3,.81),(2.24E-3,.70),(2.26E-3,.60),(2.28E-3,.50)....
          (2.30E-3,.40),(2.34E-3,.30),(2.42E-3,.20),(2.50E-3,.13)....
          (2.54E-3,.10),(2.60E-3,.07),(2.70E-3,.05),(2.80E-3,.03)....
          (2.9E-3,.025),(3.0E-3,.023),(3.2E-3,.021),(3.4E-3,.019)....
          (3.6E-3,.015),(3.8E-3,.01),(4.56E-3,1.0E-4),(5.0E-3,0.0)
          FUNCTION ADSISO=(1.0E-04,1.0E-06),(2.7E-04,2.5E-06)....
          (3.8E-04,3.5E-06),(6.8E-04,6.0E-06),(1.4E-03,1.0E-05)....
          (2.9E-03,1.9E-05),(4.3E-03,2.5E-05),(7.0E-03,3.5E-05)....
          (1.0E-02,4.4E-05),(1.9E-02,6.0E-05),(3.0E-02,7.65E-05)....
          (.068,.11E-03),(.2,.16E-03),(.45,.2E-03),(.8,.23E-03)....
          (1.0,.24E-03),(1.09,.247E-03)
DYNAMIC
          THLA=NLFGEN(TBTHLA,LAMEDA)
          SEELA=NLFGEN(TBSELA,LAMEDA)
          SS=NLFGEN(ADSISO,SEELA)
          DTHLA=DERIV(DTHLA0,THLA)
          DSEELA=DERIV(DSELA0,SEELA)
          DSS=DERIV(DSS0,SS)
          AA=INTGRL(SEE0,DSEELA)
          C=INTGRL(0.0,THLA)
          DB=INTGRL(B0,DSS)
          KON1=THETAN*LAMDAN
          E=(THLA*LAMBDA)-KON1
          FF=E-C
          G=FF+KON2
          D=-.5*G/DTHLA
          E1=LAMBDA*RHO*DSS
          LATHAD=(.5*THLA*LAMBDA+D*DTHLA)*DSEELA+(.5*E1)
          G1=INTGRL(0.0,LATHAD)
          G2=KON3-G1
          THDS=G2/DSEELA
          DS=THDS/THLA
          NOSORT
          IF(FLAG.EQ.0.AND.I.LT.2) GO TO 10
          IF(THDS.EQ.0.0) GO TO 10
          SORT
          VELK=INTGRL(VELK0,DIV)
          VELKA=INTGRL(VELKA0,DIVA)
          DIV=(-.5*THLA*LAMBDA*VELK/THDS)-(D*VELK*DTHLA/THDS)-.5*E1
          DIVA=(-.5*THLA*LAMBDA*VELKA/THDS)-(D*VELKA*DTHLA/THDS)-.5*E1
          SEE1=INTGRL(SEE0,VELK/THDS)
          SEEA=INTGRL(SEE0,VELKA/THDS)
          NOSORT
   10     CONTINUE
TERMINAL
          PRINT D,E,THLA,LATHAD,THDS,DS,SEELA,SEE1
          TIMER FINTIM=4.56E-03,PRDEL=9.12E-05,DELMIN=4.56E-20
          IF(FLAG.EQ.1) GO TO 15
          I=I+1
          KON2=C
          KON3=G1
          IF(I.GE.3) FLAG=1
          WRITE(6,100) KON2,KON3
  100     FORMAT(///' KON2,KON3=',2E15.6)
          IF(FLAG.EQ.0) GO TO 20
   15     J=J+1
          IF(ABS(SEE1-SEEN).LT.1.0E-10) STOP
          DSEE=SEEA-SEE1
          SSLOPE=DSEE/DEL/VELK0
          DRVEL=(SEE1-SEEN)/SSLOPE
          VELK0=VELK0-DRVEL
          VELKA0=VELK0*(1.0+DEL)
```

```
          WRITE(6,101) DSEE.SSLCPE.DRVEL
    101   FORMAT(///' DSEE.SSLCPE.DRVEL=',3E15.6)
          WRITE(6,102) VELKC.VELKAC
    102   FORMAT(//' CALL RERUN WITH VELKG,VELKAU=',2E20.7)
    20    IF(I.GT.10) STOP
          IF(J.GT.7) STOP
          CALL RERUN
      END
      STOP

OUTPUT VARIABLE SEQUENCE
VELKAC SEELA  DSEELA AA     THLA   C      SS     DSS    BB     E1
CTHLA  KONI   E      FF     G      D      LATHAD G1     G2     THDS
DS     ZZ0007 DIV    VELK   DIVA   VELKA  ZZ0011 SEE1   ZZ0013 SESA
ZZC014 ZZC015 I      KON2   KON3   FLAG   J      DSEE   SSLOPE DRVEL
VELKC  VELKAC

 OUTPUTS    INPUTS   PARAMS  INTEGS + MEM BLKS  FORTRAN  DATA CDS
 46(500)  107(1400)  22(400)   8+  0=  8(300)   55(600)     30

      ENDJOB
```

APPENDIX H

CSMP listing for calculating χ, ψ and ω for water and salt flow for Akuse clay

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                   ****CONTINUOUS SYSTEM MODELING PROGRAM****

                              *** VERSION 1.3 ***

     TITLE CHI,PSI, AND OMEGA FOR WATER AND SALT FLOW (AKUSE CLAY)
     *     UNITS
     *     KEQ=KILO-EQUIVALENTS
     *     KG=KILOGRAMS
     *     M=METERS
     *     S=SECONDS
     *     GLOSSARY OF SYMBOLS
     *     RVELN=PRODUCT OF SOIL WATER DIFFUSIVITY, DERIVATIVE OF WATER
     *     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF CHI OF
     *     WATER WITH RESPECT TO LAMBDA AT LAMDAN (=LAMBDA AT FINTIM)
     *     QVELN=PRODUCT OF SOIL WATER DIFFUSIVITY, DERIVATIVE OF WATER
     *     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF PSI FOR
     *     WATER WITH RESPECT TO LAMBDA MINUS Q EVALUATED AT LAMDAN
     *     (=LAMBDA AT FINTIM)
     *     Q=PRODUCT OF SOIL WATER DIFFUSIVITY ,DERIVATIVE OF WATER
     *     CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF CHI OF
     *     WATER SQUARED
     *     R=Q MULTIPLIED BY THE DIFFERENCE BETWEEN TWICE THE DERIVATIVE
     *     OF PSI FOR WATER WITH RESPECT TO CHI FOR WATER AND THE
     *     DERIVATIVE OF CHI FOR WATER WITH RESPECT TO LAMBDA
     *     QS=THE PRODUCT OF WATER CONTENT ,THE DERIVATIVE OF CHLORIDE
     *     CONCENTRATION WITH RESPECT TO LAMBDA ,AND THE DERIVATIVE
     *     OF CHI FOR SALT WITH RESPECT TO LAMBDA SQUARED
     *     RS=QS MULTIPLIED BY THE DIFFERENCE BETWEEN TWICE THE DERIVATIVE
     *     OF PSI FOR SALT WITH RESPECT TO CHI FOR SALT AND THE
     *     DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
     *     SVELN=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE
     *     OF WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
     *     OMEGA FOR WATER WITH RESPECT TO LAMBDA MINUS R EVALUATED AT
     *     LAMDAN (=LAMBDA AT FINTIM)
     *     RVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT
     *     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO LAMBDA
     *     AND THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
     *     EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
     *     QVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
     *     THE DERIVATIVE OF CHLORIDE CONCENTRATION WITH RESPECT TO
     *     LAMBDA AND THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO
     *     LAMBDA MINUS QS EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
     *     SVELNS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
     *     THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
     *     LAMBDA AND THE DERIVATIVE OF OMEGA OF SALT WITH RESPECT TO
     *     LAMBDA EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
     *     SEELAO=DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RWSPECT TO
     *     LAMBDA EVALUATED AT LAMDAN (=LAMBDA AT FINTIM)
     *     SEEO=CHLORIDE CONCENTRATION AT LAMBDA EQUALS ZERO
     *     SEEN=INITIAL CHLORIDE CONCENTRATION OF THE MOIST SOIL
     *     DCONDO=DERIVATIVE OF THE HYDRAULIC CONDUCTIVITY WITH RESPECT TO
     *     LAMBDA EVALUATED AT LAMDAN (=LAMDA AT FINTIM)
     *     RVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY,THE DERIVATIVE OF
     *     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
     *     CHI OF WATER WITH RESPECT TO LAMBDA
     *     RVELO=RVEL EVALUATED AT LAMBDA EQUALS ZERO
     *     QVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE OF
     *     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
     *     PSI OF WATER WITH RESPECT TO LAMBDA MINUS Q
     *     QVELO=QVEL EVALUATED AT LAMBDA EQUALS ZERO
     *     SVEL=THE PRODUCT OF SOIL WATER DIFFUSIVITY ,THE DERIVATIVE OF
     *     WATER CONTENT WITH RESPECT TO LAMBDA AND THE DERIVATIVE OF
     *     OMEGA FOR WATER WITH RESPECT TO LAMBDA MINUS R
     *     SVELO=SVEL EVALUATED AT LAMBDA EQUALS ZERO
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*      RVELS=THE PRODUCT OF WATER CONTENT, THE DISPERSION COEFFICIENT
*      THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*      LAMBDA AND THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO
*      LAMBDA
*      VELO=RVELS EVALUATED AT LAMBDA EQUALS ZERO
*      QVELS=THE PRODUCT OF WATER CONTENT ,THE DISPERSION COEFFICIENT,
*      THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*      LAMBDA AND THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO
*      LAMBDA MINUS QS
*      QVELOS=QVELS EVALUATED AT LAMBDA EQUALS ZERO
*      SVELS=THE PRODUCT OF THE WATER CONTENT, THE DISPERSION COEFFICIENT
*      THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT TO
*      LAMBDA AND THE DERIVATIVE OF OMEGA FOR SALT WITH RESPECT TO
*      LAMBDA MINUS RS
*      SVELOS=SVELS EVALUATED AT LAMBDA EQUALS ZERO
*      THLAO=THE DERIVATIVE OF THE WATER CONTENT WITH RESPECT TO
*      LAMBDA EVALUATED AT LAMBDA EQUALS ZERO
*      THETAO=WATER CONTENT AT LAMBDA EQUALS ZERO
*      DPSIO=THE DERIVATIVE OF PSI FOR WATER WITH RESPECT TO LAMBDA
*      EVALUATED AT LAMBDA EQUALS ZERO
*      DCHIO=THE DERIVATIVE OF CHI FOR WATER WITH RESPECT TO LAMBDA
*      EVALUATED AT LAMBDA EQUALS ZERO
*      OMEGAO=THE DERIVATIVE OF OMEGA OF WATER WITH RESPECT TO
*      LAMBDA EVALUATED AT LAMBDA EQUALS ZERO
*      DCHISO=THE DERIVATIVE OF CHI FOR SALT WITH RESPECT TO LAMBDA
*      EVALUATED AT LAMBDA EQUALS ZERO
*      DPSISO=THE DERIVATIVE OF PSI FOR SALT WITH RESPECT TO LAMBDA
*      EVALUATED AT LAMBDA EQUALS ZERO
*      KON2=THE INTEGRAL VALUE OF THE WATER CONTENT FROM LAMBDA EQUALS
*      ZERO TO LAMBDAN (=LAMBDA AT FINTIM)
*      G=THE SUM OF THETA TIMES LAMBDA AND TWICE THE SOIL WATER
*      DIFFUSIVITY MULTIPLIED BY THE DERIVATIVE OF WATER CONTENT WITH
*      RESPECT TO LAMBDA
*      KON3=THE INTEGRAL VALUE OF THE PRODUCT OF G AND THE DERIVATIVE
*      OF THE CHLORIDE CONCENTRATION WITH RESPECT TO LAMBDA FROM
*      LAMBDA EQUALS ZERO TO LAMDAN (=LAMBDA AT FINTIM)
*      THETAN=INITIAL SOIL WATER CONTENT
*      SEE=TABLE OF CHLORIDE CONCENTRATION VERSUS LAMBDA
*      THETA=TABLE OF WATER CONTENT VERSUS LAMBDA
*      COND=TABLE OF HYDRAULIC CONDUCTIVITY VERSUS WATER CONTENT
*      THLA=LINEAR INTERPOLATION OF THETA-LAMBDA EXPERIMENTAL DATA
*      PROVIDED IN FUNCTION THETA
*      SEELA=LINEAR INTERPOLATION OF EXPERIMENTAL CONCENTRATION
*      VERSUS LAMBDA DATA PROVIDED IN FUNCTION SEE
*      HCOND=NON-LINEAR INTERPOLATION OF HYDRAULIC CONDUCTIVITY
*      VERSUS LAMBDA THROUGH THE DERIVED HYDRAULIC CONDUCTIVITY VERSUS
*      THETA PROVIDED IN FUNCTION COND
*      A=DERIVATIVE OF WATER CONTENT WITH RESPECT TO LAMBDA
*      C=INTEGRAL VALUE OF THETA FROM LAMBDA EQUALS ZERO TO LAMDAN
*      (=LAMBDA AT FINTIM)
*      D=SOIL WATER DIFFUSIVITY
*      CTHETA=DIMENSIONLESS WATER CONTENT
*      CSEE=DIMENSIONLESS CHLORIDE CONCENTRATION
*      C1=THE DERIVATIVE OF THE CHLORIDE CONCENTRATION WITH RESPECT
*      TO LAMBDA
*      DS=DISPERSION COEFFICIENT
*      THDS=THE PRODUCT OF THE WATER CONTENT AND THE DISPERSION
*      COEFFICIENT
*      RDIV=THE DERIVATIVE OF Y1 WITH RESPECT TO LAMBDA IN EQUATION 4.136
*      QDIV=THE DERIVATIVE OF Y3 WITH RESPECT TO LAMBDA IN EQUATION 4.138
*      SDIV=THE DERIVATIVE OF Y5 WITH RESPECT TO LAMBDA IN EQUATION 4.140
*      RDIVS=THE DERIVATIVE OF Y2 WITH RESPECT TO LAMBDA IN EQUATION 4.137
*      QDIVS=THE DERIVATIVE OF Y4 WITH RESPECT TO LAMBDA IN EQUATION 4.139
*      SDIVS=THE DERIVATIVE OF Y6 WITH RESPECT TO LAMBDA IN EQUATION 4.141
*      CHI=CHI FOR WATER
*      PSI=PSI FOR WATER
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*    OMEGA=OMEGA FOR WATER
*    CHIS=CHI FOR SALT
*    PSIS=PSI FOR SALT
*    OMEGAS=OMEGA FOR SALT
   RENAME TIME=LAMDA
 INITIAL
         INCON DEL=.00001,RVELN=0.0,QVELN=0.0,SVELN=0.0,...
         RVELO=-.1215E-04,QVELC=.36658E-07,SVELO=.60442E-10,...
         DCHID=1.384E-02,DPSIO=1.5103E-04,DCHISO=.45815E-02
         PARAMETER THLAO=-1.0E01,J=0,THETAD=.526,I=0,KCN3=1.0,...
         SEED=.92,SEEN=.00006,SEELAD=-1.0
         CONSTANT THETAN=.10,KON2=1.0,LAMDAN=4.56E-03,...
         DCONDO=-5.1096E-03,RVELNS=0.0,QVELNS=0.0,SVELNS=0.0,...
         DPSISO=1.886E-05,OMEGAO=1.3863E-06,...
         VELO=-.32982E-06,QVELCS=.152495E-09,SVELOS=.334872E-10
         FUNCTION THETA=(0.0,.526),(1.0E-4,.525),(2.0E-4,.524),...
         (6.0E-4,.52),(1.2E-3,.515),(1.8E-3,.51),(2.2E-3,.505),...
         (2.4E-3,.504),(2.5E-3,.503),(2.6E-3,.50),(3.0E-3,.495),...
         (3.2E-3,.4875),(3.4E-3,.480),(3.5E-3,.475),(3.6E-3,.470),...
         (3.7E-3,.464),(3.8E-3,.455),(3.9E-3,.4475),(4.0E-3,.435),...
         (4.1E-3,.420),(4.2E-3,.40),(4.3E-3,.370),(4.40E-3,.33),...
         (4.46E-3,.295),(4.50E-3,.250),(4.56E-3,.10),(5.0E-3,.10)
         FUNCTION SEE=(0.0,.92),(1.0E-04,.9199),(2.0E-04,.9198),...
         (3.0E-04,.9197),(4.0E-04,.9196),(5.0E-04,.9195),...
         (6.0E-04,.9194),(7.0E-04,.9193),(8.0E-04,.9192),...
         (9.0E-04,.9191),(1.0E-03,.919),(1.1E-03,.9189),...
         (1.2E-03,.9188),(1.3E-03,.9187),(1.4E-03,.9186),...
         (1.5E-03,.9185),(1.6E-03,.9184),(1.7E-03,.9183),...
         (1.8E-03,.9182),(1.9E-03,.9181),(2.0E-03,.918),...
         (2.1E-03,.9179),(2.2E-03,.91),...
         (2.4E-03,.905),(2.6E-03,.90),(2.7E-03,.89),(2.8E-03,.88),...
         (2.9E-03,.87),(3.0E-03,.86),(3.1E-03,.84),(3.2E-03,.82),...
         (3.3E-03,.80),(3.4E-03,.77),(3.5E-03,.735),(3.6E-03,.695),...
         (3.7E-03,.645),(3.8E-03,.585),(3.9E-03,.50),(4.0E-3,.38),...
         (4.1E-03,.20),(4.12E-03,.17),(4.14E-03,.14),(4.16E-3,.12),...
         (4.18E-03,.09),(4.2E-03,.075),(4.22E-03,.06),(4.24E-3,.04),...
         (4.26E-03,.03),(4.28E-03,.02),(4.3E-03,.015),(4.34E-03,.01),...
         (4.36E-03,.008),(4.38E-03,.006),(4.4E-03,.004),...
         (4.42E-03,.002),(4.44E-03,.0009),(4.46E-03,.0007),...
         (4.4688E-03,.0006),(4.48E-03,.0005),(4.5E-03,.0003),...
         (4.52E-03,.0001),(4.54E-03,.00008),(4.56E-03,.00006),...
         (4.57E-03,.00005),(4.58E-03,.00004)
         FUNCTION COND=(.1,3.6E-08),(.1426,3.9E-08),(.1852,4.2E-08),...
         (.2278,4.8E-08),(.2704,6.0E-08),(.296,7.8E-08),(.313,1.0E-07),...
         (.33,1.4E-07),(.3471,2.0E-07),(.3556,2.5E-07),...
         (.3897,6.0E-07),(.3982,7.6E-07),(.4152,1.2E-06),...
         (.4238,1.5E-06),(.4408,2.3E-06),(.4578,3.5E-06),...
         (.4749,5.4E-06),(.4834,6.7E-06),(.4919,8.4E-06),...
         (.5175,1.6E-05),(.526,2.0E-05)
         RVELAO=RVELO*(1.0+DEL)
         QVELAO=QVELO*(1.0+DEL)
         SVELAO=SVELC*(1.0+DEL)
         VELAO=VELO*(1.0+DEL)
         QLAOS=QVELOS*(1.0+DEL)
         VELSAO=SVELOS*(1.0+DEL)
 DYNAMIC
         THLA=AFGEN(THETA,LAMDA)
         HCOND=NLFGEN(COND,THLA)
         DHCOND=DERIV(DCONDO,HCOND)
         A=DERIV(THLAO,THLA)
         C=INTGRL(0.0,THLA)
         KON1=LAMDAN*THETAN
         E=(THLA*LAMDA)-KON1
         FF=E-C
         G=FF+KON2
         D=-.5*G/A
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CTHETA=(THLA-THETAN)/(THETAO-THETAN)
CSEE=(SEELA-SEEN)/(SEEO-SEEN)
SEELA=AFGEN(SEE,LAMDA)
C1=DERIV(SEELAO,SEELA)
LATHH=(THLA*LAMDA)+(2.0*D*A)
GS=C1*LATHH
HS=INTGRL(0.0,GS)
HS1=KON3-HS
THDS=.5*HS1/C1
DS=THDS/THLA
NOSORT
IF(J.LE.3) GO TO 10
IF(THDS.EQ.0.0) GO TO 10
SORT
RDIV=(CHI*A)-DHCOND
RDIVA=(CHIA*A)-DHCOND
RVEL=INTGRL(RVELO,RDIV)
RVELA=INTGRL(RVELAO,RDIVA)
B1=RVEL/(D*A)
BB1=RVELA/(D*A)
CHI=INTGRL(0.0,B1)
CHIA=INTGRL(0.0,BB1)
DDCHI=DERIV(DCHIO,CHI)
Q=D*A*DDCHI*DDCHI
QDIV=1.5*PSI*A
QDIVA=1.5*PSIA*A
QVEL=INTGRL(QVELO,QDIV)
QVELA=INTGRL(QVELAO,QDIVA)
CC1=(QVEL+Q)/(A*D)
CC2=(QVELA+Q)/(A*D)
PSI=INTGRL(0.0,CC1)
PSIA=INTGRL(0.0,CC2)
DPSI=DERIV(DPSIO,PSI)
CC3=(2.0*DPSI/DDCHI)-DDCHI
R=Q*CC3
SDIV=2.0*OMEGA*A
SDIVA=2.0*OMEGAA*A
SVEL=INTGRL(SVELO,SDIV)
SVELA=INTGRL(SVELAO,SDIVA)
DD1=(SVEL+R)/(A*D)
DD2=(SVELA+R)/(A*D)
OMEGA=INTGRL(0.0,DD1)
OMEGAA=INTGRL(0.0,DD2)
DOMEGA=DERIV(OMEGAO,OMEGA)
RDIVS=((THLA*CHIS)-(D*A*DDCHI)-HCOND)*C1
RDIVAS=((THLA*CHIAS)-(D*A*DDCHI)-HCOND)*C1
RVELS=INTGRL(VELO,RDIVS)
RVELAS=INTGRL(VELAO,RDIVAS)
BB=RVELS/(THDS*C1)
BBA=RVELAS/(THDS*C1)
CHIS=INTGRL(0.0,BB)
CHIAS=INTGRL(0.0,BBA)
DCHIS=DERIV(DCHISO,CHIS)
QS=THDS*C1*DCHIS*DCHIS
QDIVS=((1.5*THLA*PSIS)-(D*A*DPSI)+Q)*C1
QDIVAS=((1.5*THLA*PSIAS)-(D*A*DPSI)+Q)*C1
QVELS=INTGRL(QVELOS,QDIVS)
QVELAS=INTGRL(QLAOS,QDIVAS)
CC=(QVELS+QS)/(THDS*C1)
CCA=(QVELAS+QS)/(THDS*C1)
PSIS=INTGRL(0.0,CC)
PSIAS=INTGRL(0.0,CCA)
DPSIS=DERIV(DPSISO,PSIS)
RS=QS*((2.0*DPSIS/DCHIS)-DCHIS)
SDIVS=((2.0*THLA*OMEGAS)-(D*A*DOMEGA)+R)*C1
SDIVAS=((2.0*THLA*MEGAAS)-(D*A*DOMEGA)+R)*C1
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          SVELS=INTGRL(SVELOS,SDIVS)
          SVELAS=INTGRL(VELSAO,SDIVAS)
          DD=(SVELS+RS)/(THDS*C1)
          DDA=(SVELAS+RS)/(THDS*C1)
          OMEGAS=INTGRL(0.0,DD)
          MEGAAS=INTGRL(0.0,DDA)
          NOSORT
   10     CONTINUE
 TERMINAL
          METHOD SIMP
          TIMER FINTIM=4.56E-03,PRDEL=9.12E-05,DELT=2.85E-06
          PRINT CTHETA,CHI,PSI,CMEGA,CSEE,CHIS,PSIS,OMEGAS
          IF(J.GE.4) GO TO 15
          J=J+1
          KON2=C
          KON3=HS
          GO TO 20
   15     I=I+1
          IF(ABS(RVELN-RVEL).EQ.C.0) STOP
          IF(ABS(QVELN-QVEL).EQ.0.0) STOP
          IF(ABS(SVELN-SVEL).EC.C.C) STCP
          IF(ABS(RVELNS-RVELS).EQ.0.0) STCP
          IF(ABS(QVELNS-QVELS).EQ.0.0) STCP
          IF(ABS(SVELNS-SVELS).EQ.0.0) STCP
          DVEL=RVELA-RVEL
          DVEL1=QVELA-QVEL
          DVEL2=SVELA-SVEL
          DVELS=RVELAS-RVELS
          DVELS1=QVELAS-QVELS
          DVELS2=SVELAS-SVELS
          SLOPE=DVEL/DEL/RVELO
          SLOPE1=DVEL1/DEL/QVELC
          SLOPE2=DVEL2/DEL/SVELC
          RSLOPE=DVELS/DEL/VELC
          QSLOPE=DVELS1/DEL/QVELCS
          SSLOPE=DVELS2/DEL/SVELCS
          DRVEL=(RVELN-RVEL)/SLCPE
          DQVEL=(QVELN-QVEL)/SLCPE1
          DSVEL=(SVELN-SVEL)/SLCPE2
          DRVELS=(RVELNS-RVELS)/RSLOPE
          DQVELS=(QVELNS-QVELS)/QSLOPE
          DSVELS=(SVELNS-SVELS)/SSLOPE
          RVELO=RVELO+DRVEL
          QVELO=QVELO+DQVEL
          SVELO=SVELO+DSVEL
          VELC=VELO+DRVELS
          QVELOS=QVELOS+DQVELS
          SVELOS=SVELCS+DSVELS
          RVELAO=RVELC*(1.0+DEL)
          QVELAO=QVELC*(1.0+DEL)
          SVELAO=SVELC*(1.0+DEL)
          VELAO=VELO*(1.0+DEL)
          QLAOS=QVELOS*(1.0+DEL)
          VELSAO=SVELCS*(1.0+DEL)
          WRITE(6,101) RVELO,RVELAO
  101     FORMAT(//' CALL RERUN WITH RVELC,RVELAO=',2E20.7)
          WRITE(6,102) QVELO,QVELAO
  102     FORMAT(//' CALL RERUN WITH QVELC,QVELAO=',2E20.7)
          WRITE(6,103) SVELO,SVELAO
  103     FORMAT(//' CALL RERUN WITH SVELC,SVELAO=',2E20.7)
          WRITE(6,104) VELO,VELAC
  104     FORMAT(//' CALL RERUN WITH VELO,VELAO=',2E20.7)
          WRITE(6,105) QVELOS,QLAOS
  105     FORMAT(//' CALL RERUN WITH QVELOS,QLAOS=',2E20.7)
          WRITE(6,106) SVELOS,VELSAO
  106     FORMAT(//' CALL RERUN WITH SVELCS,VELSAO=',2E20.7)
   20     IF(J.GT.15) STOP
          IF(I.GT.13) STOP
          CALL RERUN
 END
 STOP
```

APPENDIX I

CSMP listing for simulating water content profiles for various time periods for vertical infiltration of water and salt (Akuse clay)

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                  ****CONTINUOUS SYSTEM MODELING PROGRAM****

                           *** VERSION 1.3 ***

TITLE SOIL WATER CONTENT PROFILE WITH TIME (AKUSE CLAY)
*     UNITS
*     KG=KILOGRAMS
*     M=METERS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     CTHETA=DIMENSIONLESS WATER CONTENT
*     THETAC=SOIL WATER CONTENT AT LAMBDA EQUALS ZERO, CHI EQUALS ZERO,
*     PSI EQUALS ZERO, AND OMEGA EQUALS ZERO
*     THETAN=INITIAL SOIL WATER CONTENT
*     T=TIME
*     THETA=SOIL WATER CONTENT
*     LAMDA=TABLE OF LAMBDA AND CORRESPONDING WATER CONTENT VALUES
*     CHITH=TABLE OF CHI FOR WATER AND CORRESPONDING WATER CONTENT VALUES
*     PSITH=TABLE OF PSI FOR WATER AND CORRESPONDING WATEP CONTENT VALUES
   RENAME TIME=CTHETA
        INCON THETAC=.526,THETAN=.10
        PARAMETER T=(360.0,7200.0,14400.0,21600.0)
        FUNCTION LAMDA=(.1,4.56E-03),(.25,4.5E-03),...
        (.295,4.46E-03),(.33,4.4E-03),(.37,4.3E-03),...
        (.4,4.2E-03),(.42,4.1E-03),(.435,4.0E-03),...
        (.4475,3.9E-03),(.455,3.8E-03),(.464,3.7E-03),...
        (.47,3.6E-03),(.475,3.5E-03),(.48,3.4E-03),...
        (.4875,3.2E-03),(.495,3.0E-03),(.5,2.6E-03),...
        (.503,2.5E-03),(.504,2.4E-03),(.505,2.2E-03),...
        (.524,2.0E-04),(.525,1.0E-04),(.526,0.0)
        FUNCTION CHITH=(0.0,1.67E-05),(.1,1.6906E-05),...
        (.214,1.725E-05),(.3572,1.8622E-05),(.38776,1.9282E-05),...
        (.41008,1.9902E-05),(.42624,2.0469E-05),(.4448,2.121E-05),...
        (.45272,2.1628E-05),(.46047,2.1991E-05),...
        (.46986,2.2408E-05),(.47444,2.2612E-05),(.47672,2.2692E-05),...
        (.479,2.2757E-05),(.48096,2.2806E-05),(.48267,2.2841E-05),...
        (.48438,2.2863E-05),(.48609,2.287E-05),(.4878,2.2861E-05),...
        (.49122,2.2794E-05),(.50002,2.1549E-05),(.50383,2.0802E-05),...
        (.50483,1.9944E-05),(.50685,1.9008E-05),(.5097,1.7646E-05),...
        (.51094,1.673E-05),(.51284,1.5079E-05),(.51398,1.4012E-05),...
        (.51512,1.2885E-05),(.51626,1.1697E-05),(.5174,1.0448E-05),...
        (.51854,9.1309E-06),(.52007,7.2566E-06),(.52235,4.6914E-06),...
        (.52418,2.4391E-06),(.52554,6.2774E-07),(.526,0.0)
        FUNCTION PSITH=(0.0,5.7E-08),(.1,5.6914E-08),...
        (.214,5.6054E-08),(.3572,5.2574E-08),(.38776,5.1197E-08),...
        (.41008,5.0385E-08),(.42624,5.025E-08),(.4448,5.1314E-08),...
        (.45272,5.28E-08),(.46047,5.475E-08),(.46986,5.8596E-08),...
        (.47444,6.1566E-08),(.47672,6.3142E-08),(.479,6.4771E-08),...
        (.48096,6.6445E-08),(.48267,6.8146E-08),(.48438,6.9867E-08),...
        (.48609,7.1602E-08),(.4878,7.3339E-08),(.49122,7.6777E-08),...
        (.50002,9.2969E-08),(.50383,9.7054E-08),(.50483,1.0023E-07),...
        (.50685,1.0265E-07),(.5097,1.0362E-07),(.51094,1.03E-07),...
        (.51284,1.0027E-07),(.51398,9.7516E-08),(.51512,9.3829E-08),...
        (.51626,8.9138E-08),(.5174,8.3365E-08),(.51854,7.6338E-08),...
        (.52007,6.4632E-08),(.52235,4.5228E-08),(.52418,2.501E-08),...
        (.52554,6.7353E-09),(.526,0.0)
        FUNCTION MEGATH=(0.0,7.36E-11),(.1,7.3659E-11),...
        (.214,7.7917E-11),(.3572,6.5816E-11),(.38776,5.7503E-11),...
        (.41008,4.6259E-11),(.42624,3.22E-11),(.4448,7.9704E-12),...
        (.45272,-8.5632E-12),(.46047,-2.425E-11),(.46986,-4.3244E-11),...
        (.47444,-5.2214E-11),(.47672,-5.5423E-11),...
        (.479,-5.759E-11),(.48096,-5.8659E-11),(.48267,-5.8784E-11),...
        (.48438,-5.7917E-11),(.48609,-5.594E-11),(.4878,-5.2788E-11),...
        (.49122,-4.2735E-11),(.50002,7.1502E-11),(.50383,1.2717E-10)...
```

```
                 (.50483,1.8577E-10),(.50665,2.4522E-10),(.5097,3.1797E-10),...
                 (.51094,3.5849E-10),(.51284,4.1867E-10),(.51398,4.4859E-10),...
                 (.51512,4.7239E-10),(.51626,4.8869E-10),(.5174,4.9583E-10),...
                 (.51854,4.9119E-10),(.52007,4.603E-10),(.52235,3.6356E-10),...
                 (.52418,2.201E-10),(.52554,6.3216E-11),(.526,0.0)
                 THETA=CTHETA*(THETAC-THETAN)+THETAN
                 A1=NLFGEN(LAMDA,THETA)
                 A2=NLFGEN(CHITH,THETA)
                 A3=NLFGEN(PSITH,THETA)
                 A4=NLFGEN(MEGATH,THETA)
                 B1=A1*SQRT(T)
                 B2=A2*T
                 B3=A3*(T**1.5)
                 B4=A4*T*T
                 Z=B1+B2+B3+B4
                 TIMER FINTIM=1.0,PRDEL=2.0E-02,CUTDEL=4.0E-02
                 PRTPLT Z
                 LABEL MOISTURE CONTENT PROFILE WITH TIME
                 PRINT THETA,A1,A2,B1,B2,B3,B4,Z
         END
         STOP

OUTPUT VARIABLE SEQUENCE
THETA  A4      B4      A3      B3      A2      B2      A1      B1      Z

 OUTPUTS    INPUTS    PARAMS  INTEGS + MEM BLKS  FORTRAN  DATA CDS
 14(500)    43(1400)  10(400)   0+   0=  0(300)  11(600)      55


         ENDJOB
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APPENDIX J

CSMP listing for simulating concentration of Cl^- profiles for various time periods for vertical infiltration of water and salt (Akuse clay)

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                ****CONTINUOUS SYSTEM MODELING PROGRAM****

                         *** VERSION 1.3 ***

TITLE CHLORIDE CONCENTRATION PROFILES WITH TIME (AKUSE CLAY)
*     UNITS
*     KG=KILOGRAMS
*     M=METERS
*     KEQ=KILO-EQUIVALENTS
*     S=SECONDS
*     GLOSSARY OF SYMBOLS
*     CSEE=DIMENSIONLESS CONCENTRATION
*     SEEO=CONCENTRATION OF CHLORIDE AT LAMBDA EQUALS ZERO , CHI FOR
*     SALT EQUALS ZERO, PSI FOR SALT EQUALS ZERO, AND OMEGA FOR SALT
*     EQUALS ZERO
*     SEEN=INITIAL CONCENTRATION OF CHLORIDE IN THE MOIST SOIL
*     CLAMDA=TABLE OF LAMBDA AND CORRESPONDING CONCENTRATION VALUES
*     CHIS=TABLE OF CHI FOR SALT AND CORRESPONDING CONCENTRATION VALUES
*     PSIS=TABLE OF PSI FOR SALT AND CORRESPONDING CONCENTRATION VALUES
*     OMEGAS=TABLE OF OMEGA FOR SALT AND CORRESPONDING CONCENTRATION
*     VALUES
*     T=TIME
*     SEE=CONCENTRATION OF CHLORIDE IN SOLUTION
  RENAME TIME=CSEE
          INCON SEEO=.92,SEEN=.00006
          PARAMETER T=(3600.0,7200.0,14400.0,21600.0)
          FUNCTION CLAMDA=(.00004,4.58E-03),(.00005,4.57E-03),...
          (.00006,4.56E-03),(.00008,4.54E-03),(.0001,4.52E-03),...
          (.0003,4.5E-03),(.0005,4.48E-03),(.0006,4.4688E-03),...
          (.0007,4.46E-03),(.0009,4.44E-03),(.002,4.42E-03),...
          (.004,4.4E-03),(.006,4.38E-03),(.008,4.36E-03),...
          (.01,4.34E-03),(.015,4.3E-03),(.02,4.28E-03),(.03,4.26E-03),...
          (.04,4.24E-03),(.06,4.22E-03),(.075,4.2E-03),(.09,4.18E-3),...
          (.12,4.16E-03),(.14,4.14E-03),(.17,4.12E-03),(.2,4.1E-03),...
          (.38,4.0E-03),(.50,3.9E-03),(.585,3.8E-03),(.645,3.7E-03),...
          (.695,3.6E-03),(.735,3.5E-03),(.77,3.4E-03),(.8,3.3E-03),...
          (.82,3.2E-03),(.84,3.1E-03),(.86,3.0E-03),(.87,2.9E-03),...
          (.88,2.8E-03),(.89,2.7E-03),(.9,2.6E-03),(.905,2.4E-03),...
          (.91,2.2E-03),(.9179,2.1E-03),...
          (.918,2.0E-03),(.9181,1.9E-03),(.9182,1.8E-03),...
          (.9183,1.7E-03),(.9184,1.6E-03),(.9185,1.5E-03),...
          (.9186,1.4E-03),(.9187,1.3E-03),(.9188,1.2E-03),...
          (.9189,1.1E-03),(.919,1.0E-03),(.9191,9.0E-04),...
          (.9192,8.0E-04),(.9193,7.0E-04),(.9194,6.0E-04),...
          (.9195,5.0E-04),(.9196,4.0E-04),(.9197,3.0E-04),...
          (.9198,2.0E-04),(.9199,1.0E-04),(.92,0.0)
          FUNCTION CHIS=(6.0E-05,1.2584E-05),(1.5603E-04,1.2924E-05),...
          (.011,1.3373E-05),(.0396,1.3501E-05),(.1304,1.3579E-05),...
          (.27488,1.3619E-05),(.47408,1.362E-05),(.55916,1.3591E-05),...
          (.62148,1.3542E-05),(.6938,1.3433E-05),(.73052,1.3337E-05),...
          (.74704,1.3281E-05),(.763,1.3221E-05),(.77768,1.3155E-05),...
          (.79136,1.3083E-05),(.80336,1.3006E-05),(.81248,1.2924E-05),...
          (.8216,1.2838E-05),(.83984,1.265E-05),(.90002,1.1229E-05),...
          (.90458,1.0577E-05),(.90914,9.8898E-06),(.91795,9.1345E-06),...
          (.91818,8.1404E-06),(.91831,7.5422E-06),(.91854,6.5417E-06),...
          (.91868,5.9392E-06),(.91881,5.3348E-06),(.91895,4.7284E-06),...
          (.91909,4.1199E-06),(.91922,3.5092E-06),(.91941,2.6912E-06),...
          (.91964,1.6623E-06),(.91982,8.3371E-07),(.91995,2.0892E-07),...
          (.92,0.0)
          FUNCTION PSIS=(6.0E-05,4.15E-08),(1.5603E-04,5.5722E-08),...
          (.011,4.1884E-08),(.0396,4.1956E-08),(.1304,4.2167E-08),...
          (.27488,4.2398E-08),(.47408,4.2756E-08),(.55916,4.2993E-08),...
          (.62148,4.3224E-08),(.6938,4.3545E-08),(.73052,4.3733E-08),...
          (.74704,4.3815E-08),(.763,4.3888E-08),(.77768,4.3949E-08),...
```

```
         (.79136,4.3997E-08),(.80336,4.4031E-08),(.81248,4.4051E-08),...
         (.8216,4.4056E-08),(.83984,4.4011E-08),(.90002,4.184E-08),...
         (.90458,4.0158E-08),(.90914,3.8194E-08),(.91795,3.56E-08),...
         (.91818,3.1879E-08),(.91831,2.9627E-08),(.91854,2.5836E-08),...
         (.91868,2.3538E-08),(.91881,2.1218E-08),(.91895,1.8876E-08),...
         (.91909,1.6509E-08),(.91922,1.4117E-08),(.91941,1.0885E-08),...
         (.91964,6.7719E-09),(.91982,3.4166E-09),(.91995,8.6009E-10),...
         (.92,0.0)
         FUNCTION OMEGAS=(6.0E-05,3.1871E-08),(1.5603E-04,3.8004E-10),...
         (.011,5.9927E-11),(.0296,5.455E-11),(.1304,5.3146E-11),...
         (.27488,5.2527E-11),(.47408,5.2089E-11),(.55916,5.2003E-11),...
         (.62148,5.2065E-11),(.6938,5.2509E-11),(.73052,5.3079E-11),...
         (.74704,5.3452E-11),(.763,5.3886E-11),(.77768,5.4385E-11),...
         (.79136,5.4942E-11),(.80336,5.5558E-11),(.81248,5.6219E-11),...
         (.8216,5.6922E-11),(.83984,5.8448E-11),(.90002,6.6753E-11),...
         (.90458,6.8032E-11),(.90914,6.828E-11),(.91795,6.5609E-11),...
         (.91818,5.9841E-11),(.91831,5.627E-11),(.91854,5.0099E-11),...
         (.91868,4.6241E-11),(.91881,4.2244E-11),(.91895,3.8091E-11),...
         (.91909,3.3779E-11),(.91922,2.9296E-11),(.91941,2.3025E-11),...
        (.91964,1.4682E-11),(.91982,7.5599E-12),(.91995,1.9325E-12),...
         (.92,0.0)
         SEE=CSEE*(SEEO-SEEN)+SEEN
         A1=NLFGEN(CLAMDA,SEE)
         A2=NLFGEN(CHIS,SEE)
         A3=NLFGEN(PSIS,SEE)
         A4=NLFGEN(OMEGAS,SEE)
         B1=A1*SQRT(T)
         B2=A2*T
         B3=A3*(T**1.5)
         B4=A4*T*T
         Z=B1+B2+B3+B4
         TIMER FINTIM=1.0,PRDEL=2.0E-02,OUTDEL=4.0E-02
         PRTPLT Z
         LABEL CONCENTRATION PROFILE WITH TIME
         PRINT SEE,A1,A2,B1,B2,B3,B4,Z
     END
     STOP

OUTPUT VARIABLE SEQUENCE
SEE     A4      B4      A3      B3      A2      B2      A1      B1      Z

 OUTPUTS    INPUTS   PARAMS  INTEGS + MEM BLKS  FORTRAN  DATA CDS
 14(500)   43(1400)  10(400)   0+   0=  0(300)   11(600)     67

     ENDJOB
```