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# **SOIL MOISTURE REDISTRIBUTION MODELING WITH ARTIFICIAL NEURAL NETWORKS**

by  
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## ABSTRACT

This study sought to investigate the application of artificial neural networks (ANN) and fuzzy inference systems (FIS) to variably saturated soil moisture (VSSM) redistribution modelling. An enhanced approach to such modelling, that lessens computation costs, facilitates input preparation, handles data uncertainty, and realistically simulates soil moisture redistribution, was our main objective.

An initial review of existing soil hydrology models provided greater insight into current modelling challenges and a general classification of the models. The application of AI techniques as alternative tools for soil hydrology modelling was explored.

A one-dimensional (1D) model based on ANN and FIS was developed. To estimate fluxes more accurately, multiple ANNs were trained and combined by way of an FIS. The main body of the model employed the ANN-FIS module to model soil moisture redistribution throughout the profile. When tested against the SWAP93 model, the ANN-FIS model gave a good match and maximum error of <8%; however, it did not show a notable computation cost shift.

The investigation proceeded with development of another ANN-based 1D modelling approach. This time, the soil profile or flow region, regardless of its depth, was divided into ten equal parts (compartments). The ANN was trained to estimate moisture patterns for a whole soil profile, from the previous day's soil moisture pattern and boundary conditions, and the current day's boundary conditions. The model was tested against SWAP93 where an average SCORE of 90.4 indicated a good match. The computation cost of the ANN-based model was about one-third that of SWAP93.

At this point the study sought to develop a 3D modelling approach. The ANN was trained to estimate the nodal soil moisture changes through time under the

influence of six neighbouring nodes (in a 3D space, two on each axis). The model's accuracy was tested against the SWMS-3D model. An average SCORE of 91 and a 15-fold decrease in computation costs showed a quite acceptable performance. Results suggest that this approach is potentially capable of realistically modelling 3D VSSM redistribution with less computation time.

Finally, pros and cons of these ANN-based modelling approaches are compared and contrasted, and some recommendations on future work are given.

## RESUMÉ

Cette étude vise à investiguer l'enquête de l'application de réseaux neuronaux artificiels (RNA) et de systèmes d'inférence floue (SIF) à la modélisation de l'évolution du profil hydrique du sol sous des conditions de saturation variable. Une approche améliorée à cette modélisation qui réduirait les coûts de calcul, faciliterait la préparation de données, pourrait tenir compte de leur incertitude, et simulerait de façon réaliste l'évolution du régime hydrique du sol, est le principal objectif.

Une étude des présents modèles de régime hydrique du sol nous a permis une compréhension plus approfondie des présents défis de modélisation et une classification générale des modèles. L'application de techniques d'intelligence artificielle comme alternatives de modélisation pour le régime hydrique du sol a été explorée.

Un modèle unidimensionnel (1D) à base de RNA et de SIF a été développé. Afin de mieux évaluer l'évolution du profil hydrique, plusieurs RNA ont été entraînés et combinés grâce au SIF. Le module RNA-SIF représenta la plus grande partie du modèle consacrée à modéliser le régime hydrique du sol à travers le profil du sol. Lorsque comparé au modèle SWAP93, le modèle RNA-SIF corresponda bien, avec une erreur maximale inférieure 8%. Cependant, les coûts de calcul n'ont pas été réduits de façon appréciable.

L'étude continua avec le développement d'une autre approche de modélisation 1D à base de RNA. Cette fois-ci, le profil du sol ou la région d'écoulement a été divisée en 10 parties (compartiments) égales, peu importe la profondeur du profil. La RNA fut entraînée à estimer le profil hydrique de tout un profil à partir de celui du jour précédant et des conditions limites du jour précédant et du jour présent. Le modèle fut comparé au modèle SWAP93 et reçu un SCORE de

90.4, indiquant une bonne correspondance. Les coûts de calcul furent environ le tiers de ceux pour SWAP93.

L'étude visa alors le développement d'une modélisation 3D. La RNA fut entraînée à simuler l'évolution dans le temps de la teneur en eau à différents noeuds, sous l'influence des six noeuds les plus rapprochés (dans une espace 3D, deux noeuds par axe). L'exactitude du modèle fut évalué par rapport au modèle SWMS-3D. Un SCORE de 91 et des coûts de calcul quinze-fois moins élevés représentent une très bonne performance. Nos résultats suggèrent que cette approche a le potentiel de permettre une simulation réaliste et plus rapide de l'évolution du régime hydrique du sol sous des conditions de saturation variable.

Finalement, les avantages et désavantages de l'utilisation de la modélisation par RNA sont comparés et contrastés, et des recommandations pour les recherches futures sont énoncées.



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## **GUIDE LINES FOR A MANUSCRIPT BASED THESIS**

This thesis has been prepared in accordance with the February, 1999 revision of the Guidelines for Thesis Preparation (Faculty of Graduate Studies and Research, McGill University). It is stated therein that:

“As an alternative to the traditional thesis format, the dissertation can consist of a collection of papers that have a cohesive, unitary character making them a report of a single program of research.”

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“ ... In general, when co-authored papers are included in a thesis the candidate must have made a substantial contribution to all papers included in the thesis. In addition, the candidate is required to make an explicit statement in the thesis as to who contributed to such work and to what extent. This statement should appear in a single section entitled ‘Contribution of Authors’ as a preface to the thesis.”

## **CONTRIBUTION OF AUTHORS**

In accordance with the McGill “Guidelines for a Manuscript Based Thesis”, the contributions of the candidate and the co-authors towards the completion of this thesis work are set down here.

Development of the concepts, creation of the algorithms, coding of computer programs, and compilation of the simulations, was the sole responsibility of the candidate. Chapters two through five of this thesis were co-authored by the candidate, Dr. R.B. Bonnell, and Dr. S.O. Prasher. The co-authors guided the candidate towards depth and clarity in the presentation of material. These chapters are being prepared to be submitted for publication.

Other chapters were authored by the candidate. The original documentation and the creation of associated diagrams for this thesis was the responsibility of the candidate. Content of this thesis was thoroughly critiqued and reviewed by the thesis supervisor.

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## CHAPTER ONE: GENERAL INTRODUCTION

The study reported in this thesis is an exploration of an alternative simulation modeling approach for variably saturated soil moisture redistribution; which employs two artificial intelligence techniques, namely artificial neuronets and fuzzy inference systems. The adopted alternative approach is of empirical nature, rather than mechanistic. This chapter attempts to provide a background to the reader on how the study was initiated. It explains the importance of simulation models, discusses the problems associated with conventional modeling approaches, introduces the alternative approach that was developed during the course of this study, and presents a list of study objectives.

### SIMULATION MODELING

Emergence of computers in the middle of 20<sup>th</sup> century has revolutionized engineering, including Agricultural and Environmental System (AES) engineering. Combining expert knowledge of Soil Hydrology Processes (SHP) with the power of computers has led to development of many simulation models. With the ever increasing power of computers and innovations in numerical methods, SHP simulation models have been ever-rapidly evolving during the last thirty years.

During the last decade some critiques were issued on SHP models, which questioned their reliability and inherent limitations<sup>10</sup>. These critiques, emphasised the originality of physical experiments and were oriented toward a growing gap seeming to exist between computer simulations and the physical sense of a real phenomenon. While model caveats are real, it still seems that SHP simulation models are tools potentially capable of helping researchers expand their understanding of real world processes in new and efficient ways. SHP

simulation models continue to be re-examined and refined through model verification against field observations.

It is perceived by most modellers, that some understanding of real system behaviour can be achieved through less costly modelling exercises rather than by traditional field work and/or lab experimentation<sup>9</sup>. In essence, this is a valid conclusion, but it is necessary to note that as of yet nothing can completely replace field observations. At the same time, it cannot be denied that end-users of simulation models, who usually are not fully aware of model assumptions and limitations, may misuse or abuse models and/or modelling results. Although, this fact cannot be counted as a demerit point for simulation models, it should be regarded as a warning that directs modellers to provide transparent and all-inclusive information to users.

Generally speaking, SHP modelers have been successful in developing faster and more comprehensive models. Simulation models have expanded the decision-making abilities of AES engineers toward stronger environmental accounting and more comprehensive project planning. These models empower AES engineers to assess different planning/designing/operating scenarios for projects with much less effort and to get more insight into the probable consequences of each scenario. This eventually minimizes the rise of possible drawbacks and maximizes the expected benefits of the project. However, existing SHP simulation approaches still suffer from some problems and there is need for improvement. Some of these problems which fall within the scope of this study are discussed below.

### **VARIABLY SATURATED SOIL MOISTURE REDISTRIBUTION**

Many SHP deal with Variably Saturated Soil Moisture (VSSM), for instance: drainage, infiltration/seepage, and soil surface evaporation. There are various examples of simulation cases, which are based on these VSSM processes. Some



examples are: root zone moisture loss through bare soil evaporation and plants transpiration, contaminant transport and degradation in the vadose zone, and design of clay barriers for waste disposal sites. Inasmuch as VSSM redistribution is a key sub-process of many SHP, a realistic simulation of these processes requires a reliable VSSM redistribution module.

Human knowledge of VSSM was first expressed as a mathematical formula by Buckingham<sup>5</sup> in 1907. He introduced the concept of the “unsaturated hydraulic conductivity function” and modified the well known Darcy's equation to describe steady-state unsaturated flow<sup>8</sup>. Richards<sup>11</sup> formulated a general non-linear parabolic partial differential equation (pde) to represent the non-steady-state movement of water in an unsaturated soil. The non-linearity of pde is due to the fact that its coefficients (unsaturated hydraulic conductivity or differential soil moisture capacity) are functions of the dependent variable (i.e.; water potential, or moisture content). Moreover, Richards equation is a stiff\* pde, because the rate of change of 'hydraulic conductivity' and that of 'hydraulic head' are quite different. In a general three-dimensional (3D) form, Richards' equation describes VSSM flow in an anisotropic and non-homogeneous soil matrix. Inasmuch as it is a mechanistical model, its usage may be extended to any fluid flow within a porous medium, or even to multi-phase flow cases. Most existing VSSM simulation models are based on numerical (Finite Difference or Finite Element techniques) solutions of the Richards' equation. These models usually suffer from laborious programming efforts and high computation cost, especially for 3D cases<sup>2</sup>.

Natural soil is a porous system with spatio-temporal variabilities. VSSM redistribution is a natural process that intensifies the variabilities of the soil porous system. Spatial non-uniformity of the soil moisture domain yields a

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\* A differential equation is called stiff when any two —or more— of its solution components has very different time scales. That is: the rate of growth or decay of the two components are very different<sup>3</sup>.

higher non-uniformity in the unsaturated hydraulic conductivity domain. Simulation modelling of 3D VSSM is a requisite in dealing with spatial variabilities both on the field surface and through the soil profile. The spatial variabilities when aggregated with the temporal variabilities introduce high data uncertainty. Some common instances of observed data with high field and/or seasonal variabilities (that causes high variance and high data uncertainty) are unsaturated hydraulic conductivity, infiltration rate, and macro-pores (size and shape). It is essential to appreciate the fact that data uncertainty for measured (or estimated) field scale soil characteristics is inherent and unavoidable. Uncertainty is originally related to natural complexity and spatial-temporal variabilities of real soil systems and processes. In addition, with computer models, other sources of uncertainty should be taken into account. Three such sources may be named as: model simplifications / inadequacies, model parameter estimation, and flow domain / time span discretization. The last source only can be avoided if an analytical model is employed. The first and second source are inherent to any mathematical model or any simulation model based on them. Inasmuch as conventional simulation models are associated with such sources of uncertainty, their results can only be regarded as rough approximations of the real system behaviour. The alternative approach, addressed in this thesis, is aimed at elimination of the first and second sources of uncertainty mentioned above.

## **EMPIRICAL VS MECHANISTIC**

Engineering has two faces: scientific and pragmatic. Engineering as a pragmatic art is practical and aimed at solving daily problems man is faced with; however, engineering as a science is committed to exactness and is aimed at finding the truth of phenomena. Moreover, as a pragmatic art it is rooted in historical experiences (trial-error) and is empirically based; however, as a science it is rooted in scientific method (analysis-synthesis) and is mechanistically based. A

pragmatic engineer uses science but only to fulfill his duties, by taking advantage of everything that seems applicable to his profession. He is only interested in those scientific results which he considers most practical and leaves the rest for scientists<sup>4</sup>.

Most existing SHP simulation approaches during their course of evolution have embraced more and more scientific detail and gradually have become good research tools. These models usually need several input parameters which may be measured and collected, but this measurement consumes time and financial resources. There are a few simulation models, such as DRAINMOD<sup>12</sup>, which are partly based on empirical approaches. While the results of these models are quite comparable with the latter, they are usually more simple (i.e.; more lucid code, less input) and have less computation cost.

Most current scientific simulation models are mechanistic and need predefined mathematical models as their base. Besides, mathematical models are only our abstractions of real systems and do not, necessarily, include all details of the system. In fact, an ideal mathematical model that truthfully expresses the VSSM of a soil matrix, including its variabilities, has yet to be developed. Until then, the most trustworthy representation of real systems is our observations as hard (numeric) or soft (linguistic) data. When mathematical models are used, some facts about the real system will be lost. At least two reasons can be claimed for this loss. Firstly, the real system is impelled to fit in an imperfect predefined mathematical model. Secondly, mathematical models cannot receive soft data; therefore, qualitative information may not be used.

To comply with the aforementioned uncertainties, VSSM field scale (3D) input data have to be treated as functions of time and space<sup>7</sup>. The major current routine for introduction of spatio-temporal variabilities of VSSM input data into a mathematical model is to consider the data as stochastic quantities. Such an inclusion of the variabilities into mathematical models increases the computation

cost. Instead of being used as a direct design tool, the simulation models can be best used as subsets of a Decision Support System (DSS). This situation gives rise to a dilemma; on one hand, DSS requires many runs of a simulation model; and on the other hand, computation cost is high. This is a serious barrier in applicability of conventional 3D VSSM redistribution simulation models.

The alternative simulation modeling approach, as addressed in this thesis, does not need a predefined mathematical model and requires fewer inputs. The approach also has the potentiality to receive soft data and to deal with data uncertainty. As described in the next section, such an approach utilizes artificial intelligence techniques and provides a more efficient routine for information abstraction obtained from the observations.

## **ARTIFICIAL INTELLIGENCE**

There is a need for a 3D unsteady VSSM redistribution simulation model, that overcomes the pitfalls discussed above. Such a model would bestow upon engineers the ability to more realistically and easily simulate SHP. Field scale simulation of 'salt accumulation at the soil surface' or 'salt leach-out from the soil profile' under uneven topography with soil heterogeneities is an instance; where ignorance of spatial variabilities may lead to unreliable results.

There are a number of novel problem solving methodologies (e.g., Fractals, Expert Systems, Fuzzy Logic, Artificial NeuroNets) that can help SHP modellers to deal with the above mentioned difficulties. This study has employed Fuzzy Logic and Artificial NeuroNets to model VSSM redistribution.

Fuzzy logic has provided a new way to deal with the vagueness and uncertainty of real world data. Bardossy and Duckstein<sup>1</sup> have described fuzzy rule-based modelling as a new way to model complex physical processes of the real world. They were the first modellers who applied fuzzy rule-base techniques to SHP modelling. The current study has also applied fuzzy logic in the form of a fuzzy

inference system (FIS) to deal with data uncertainty and the complexity of real VSSM problems.

Artificial NeuroNets (ANN) are able to capture knowledge that is vague, complex, and not explicitly expressed by mathematical or symbolic (e.g., rule-based) means<sup>6</sup>. It is a 'data-driven' and 'predefined-model free' simulation tool that enables us to efficiently extract information from the observed data. The approach addressed in this study has employed ANN, and has achieved a much lower computation cost. The approach did not require unsaturated hydraulic conductivity as an input data. Integration between ANN and FIS helped the model to overcome data uncertainty and enhanced its output.

## **STUDY GOAL AND OBJECTIVES**

The goal of this study was to develop a 3D VSSM redistribution simulation modelling approach that employs artificial neuronet.

The thesis objectives were:

To explore applicability of ANN and FIS to unsteady VSSM redistribution simulation modelling via development of unsteady state VSSM redistribution simulation modeling approaches, in two folds for:

- One dimensional flow domain; and
- Three dimensional flow domain.

Specific to ANN and FIS application objectives were:

1. To decrease computation cost of the 3D model in comparison to conventional numerical models;
2. To simplify the model input requirements via elimination of some inputs, or substitution of some others by more simple input data; and
3. To increase the quantity of information abstraction obtained from observed data via use of ANN.

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## **CONNECTING TEXT: CHAPTERS ONE & TWO**

Chapter one, the general introduction of the thesis, gave some ideas on how this study started. Concerns on limited abilities of customary VSSM redistribution simulation models, specially about 3D models were briefly discussed. Possible utilization of AI technologies were mentioned and at the end section, the study objectives are listed. The main goal of this study is named as: exploring applicability of ANN and FIS for unsteady VSSM redistribution modelling in order to develop an ANN-based 3D simulation approach.

Chapter two serves the thesis as a literature review. It is a review on existing SHP modeling approaches which is concluded with a classification of these approaches. Inasmuch as the approach proposed (on modeling of VSSM redistribution) in this thesis is novel, no literature was found on this specific domain; however, relevant literatures (i.e., on any application of AI components to SHP) were reviewed.

## **CHAPTER TWO: A REVIEW OF THE EXISTING MODELING APPROACHS**

**ABSTRACT:** Existing approaches in variably saturated soil moisture (VSSM) movement modeling, with an emphasis on the recent trends, are reviewed in this chapter. The review is presented in a brief format and has considered the models in three parts: classical approaches, alternative approaches, and approaches based on two artificial intelligence techniques, namely fuzzy logic and artificial neuronets. In a general view, classification of models along with pros and cons of different categories is discussed. The chapter ends with a short conclusion.

### **INTRODUCTION**

During the last four decades computer simulation models have played an increasingly important role in the study of agricultural and environmental systems (AES). Since then, model limitations, reliability flaws, and their misuse have inspired some sagacious critiques on AES modeling practices<sup>60,100,135</sup>. In fact, when used properly, models are capable tools that help researchers expand our understanding of AES. Compared to field/laboratory experiments, modeling is quick and inexpensive<sup>72,91</sup>. Of course, they cannot completely substitute expensive and time consuming physical (field/laboratory) experiments. But, models can lower, to a large extent, the number of real-life experiments needed for a given research project, provided that they are considered in the “experimental design”. Moreover, by enabling us to perform several simulations, models provide more insight into the phenomena and the way different combinations of variables and parameters influence the results<sup>60,91</sup>. Generally speaking, models are helpful, powerful tools for predictive and decision-making processes, if used cautiously and knowingly.

Modeling of soil hydrology processes (SHP), a major component of an AES, has been at the center of attention of soil hydrologists for many years. Models have

been continuously evolving since the start of the computer era in SHP modeling. Use of modeling has changed our perception of soils. From a simple detachable sub-system with static parameters; we now conceive soils as an open, dynamic and heterogeneous system, which is an integral part of a continuous environment<sup>2,60,69,94</sup>. Its parameters are uncertain and have spatio-temporal variability originated by stochastic/deterministic causes<sup>72,99</sup>.

In an effort to achieve a “perfect model”, numerous models have been developed and many of these have undergone several successive improvements. Their evolutions have proceeded through several upgrading pathways: from empirical to mechanistical formulations, from time-invariant to time-variant conceptualizations, from one- to multi-dimensional models, from single- to multi-process simulations, from simple to advanced computation algorithms, and from confusing codes to more structured/modular and lucid codes. In other words, the desire to model reality as precisely as possible, has motivated modelers to develop more comprehensive and complex, yet structured models.

Complex (multi-process / multi-dimensional / mechanistical) models have inherent problems<sup>2,60</sup>. One such problem is the need for large input data sets, while at the same time, physical, expense, and time limitations oblige us to use estimates of these parameters. Tedious programming efforts and high computational costs are two other problems. More important, complex models suffer from inherent accuracy limitations<sup>10,45</sup>. That is, inasmuch as factual values of many parameters are not known, errors are introduced to the models via estimated values. Also, parameters spatio-temporal variations, which are not easy to capture minutely, contribute to the total input error to these complex models. That is not to say they are useless, but they have failed to serve us as “perfect models”. Yet, complex models can promote our insight into different cases if they are used wisely. It is interesting to note that verification and

validation of these models is impossible<sup>94</sup>. Hence, veracity and reliability of these models are unknown.

Variably-Saturated Soil-Moisture (VSSM) movement has a key role in many SHP<sup>38</sup>. For example without knowing the moisture content/potential/spatial-variation, we are not able to model solute transport. Obviously, VSSM model inaccuracies would affect, in turn, the veracity of other SHP models. Infiltration, evaporation from bare soil, evapotranspiration, redistribution, preferential flow, deep percolation, crop root development and root uptake of water are different components of VSSM models. Richards' Partial Differential Equation (PDE) is customarily used, via numerical modeling techniques (such as Picard's or Newton's), to integrate most of these components. This PDE shows high non-linearity since its coefficient, the hydraulic conductivity ( $K(h)$ ), is a nonlinear function of the soil water pressure head<sup>73</sup>. In "far from equilibrium" real situations, where flow region parameters are highly variable, spatially and/or temporally, solution of this PDE is not easy. This approach is even more complicated for multi-dimensional and for very dry cases. The aforementioned is a likely reason why most popular VSSM models are still one-dimensional.

In order to resolve the problems of complex models, a shift in our approach to VSSM modeling seems necessary. Needed are models with shorter execution times, to be used for optimization tasks; and models with much more lucid codes. To-date our customary approach is to interpret VSSM as a deterministic phenomena. However, the recognized high non-linearity of the VSSM components (both in reality and in a model) suggests the possible chaotic behavior of these phenomena<sup>239</sup>. Therefore, a new approach based on chaos theory may be more fruitful. In fact, the shift has already started. New schools of VSSM modeling, here called alternative models, have arisen. These alternative models are usually based on some new computational technique such as: fractals, artificial neuronets, fuzzy logic/mathematics, and rule bases.

This paper focuses on VSSM models and their components, browses through different types of VSSM models, both customary and alternative, with an emphasis on the most recent ones. Then a classification of VSSM models is presented, which is done through consideration of differences among models on the basis of the conceptualization, the formulation and the algorithm used. Finally, an alternative approach, that utilizes Artificial NeuroNet (ANN) and Fuzzy Inference System (FIS) technologies, is introduced.

## **A REVIEW OF VSSM MODELS**

Many attempts have been executed to model VSSM via several approaches. Most of these have used various numerical methods to solve the VSSM governing PDE, Richards' equation. Some other models have used simplified forms of this PDE, to accede analytically solvable equations. A third class may be named "conceptual models" such as multi-reservoir conceptual models, based on balance equations.

Accepting SHP complexities, as discussed earlier, modelers have tried to cope with this fact. One issue was the inherent uncertainty associated with the complex system's parameters. To embed this uncertainty into VSSM models, some modelers have treated the flow parameters as stochastic variables. Others have tried alternative approaches. A selective review of VSSM modeling efforts is given here in two parts. First, classical approaches are reviewed, and then alternative approaches are introduced.

### **Classical Approaches**

Computer simulations via numerical solutions of Richards' PDE were the most popular taken among classical approaches. The first VSSM models developed during the early sixties were based on the Finite Difference (FD) method (e.g., Hanks and Bowers<sup>52</sup>); and followed, only one decade later, by the Finite Element (FE) method (e.g., Bruch and Zyvoloski<sup>17</sup>). The most notable advantage of FE

over FD is the capability to accurately map irregular system boundaries in multi-dimensional simulations, as well as to more easily include non-homogeneous medium properties<sup>92</sup>. Yet, in terms of numerical stability and accuracy of the solutions, it has been shown for one-dimensional unsaturated flow, that FD methods are preferred over FE methods<sup>19</sup>. Celia et al.<sup>19</sup> showed that a mixed form of the Richards' equation is a general mass conservative numerical solution for VSSM flow. Some selected VSSM modeling examples from the 80s follows.

Faced with numerical problems to solve 1D Richards' equation via a FD scheme, Dane and Mathis<sup>33</sup> developed the 'space step size adaptive' scheme. Meaning that, a fixed number of nodes were automatically redistributed to establish fine grids where large soil moisture pressure head gradients occur. Moldrup et al.<sup>88</sup> promoted a rapid and numerically stable method that had been first proposed by Wind and van Doorne<sup>139</sup>. The model was labeled: the moving mean slope, because the model uses the average slope of natural log of hydraulic conductivity. Despite promising features, the model had two shortcomings: it was developed for 1D cases only, and for coarse soils it was not rapid any more.

Jensen<sup>66</sup> and Ammentorp et al.<sup>5</sup> reported their work on the unsaturated zone component of the SHE (Système Hydrologique Européen) watershed scale model. The VSSM flow component, based on one-dimensional (1D) numerical solution of Richards' equation, deals with heterogeneity through separate model runs for each typical soil profile. Another watershed model with a pioneer 3D VSSM component in its time, based on FD solution of the Richards' equation, was developed by Al-Soufi<sup>3</sup>. Inasmuch as the model was 3D, soil heterogeneities, were directly taken care of. Both models did not consider any measures for data uncertainty. To express soil data uncertainties, Chung and Austin<sup>27</sup> used stochastic inputs for their 1D model. The model considers a heterogeneous layered soil profile, and uses Monte Carlo simulation to produce stochastic input parameters for each soil layer, including hydraulic conductivity.

A comprehensive review of soil water dynamics modeling in the unsaturated zone was presented by Feddes et al.<sup>43</sup>. To know more on modeling practices before 1988 one may refer to this article. No such review has been published since 1988, however number of novel approaches and new models proposed and developed for VSSM flow from then has increased rapidly.

During the last decade, many modelers have developed their own versions of numerical computer simulation models, each with its pros and cons. They have dealt with VSSM modeling complications (soil-water nonlinear dynamics, soil-plant-atmosphere continuum, ...) in different ways. One noteworthy model (even if not a computer simulation model) in this decade is the electrical analog proposed by Hillel<sup>59</sup>. It is a didactic tool that helps to conceptualize the soil-plant-atmosphere as an integrated system and presents the complexities of such a system very well.

Some examples of more general models are: PESTFADE<sup>30</sup>, SESOIL<sup>58</sup> and UNSATCHEM<sup>121</sup>. However, many others developed models specifically aimed at certain cases or sites. These have not received the same publicity/attention as more general approaches. Innovative numerical models use approaches that have never been used earlier in VSSM modeling. An example is the model developed by Rieder and Prunty<sup>103</sup>. The model, based on a simple coupled differential equation set, solves heat and mass transfer instantaneously. Another example is the model based on the "Lie group" method of differential equations classification<sup>9</sup>. In recent years as the parallel processing becomes more available the number of VSSM models that make use of this advantage has increased. The model developed by Thomas and Li<sup>127,128</sup> is an example of such models. To attenuate the numerical difficulties, Prevedello et al.<sup>101</sup> introduced "gravitational" and "global" soil moisture diffusivities that substitutes the Richards' equation for vertical flow with a diffusivity type equation for which many solutions are available. However, their model is not applicable to a

positive pressure (saturation), which is a commonly occurring situation (infiltration/water-table). Also, in the same direction, to lessen the nonlinearity of the VSSM flow, Amokrane and Villeneuve<sup>6</sup> used a variable transformation, which reduces the Richards' equation into a diffusion format. But, inasmuch as this model is a diffusion type, as well as the other model just mentioned above, it is not applicable to saturated cases. To speed up computations a number of modelers have tried to establish more accurate explicit numerical methods, usually using a kind of predictor-corrector scheme.

Some well-known VSSM 1D models based on FD methods are LEACHM<sup>64</sup>, SWAP<sup>132</sup>, RZWQM<sup>79</sup>, Opus<sup>117</sup> and GLEAMS<sup>75</sup>. Each of these models has a long history of improvements. For instance SWAP, a new version of SWACROP and SWATRE, has been improved by a change of Richards' equation solution scheme from "head-based" to "mixed-based" due to the recommendations of Celia et al.<sup>19</sup>. Also, it has been improved by the addition of new components such as adsorption-decomposition of solutes and heat transfer; as well as by attachment of hysteresis to the water retention function<sup>132</sup>. The GLEAMS model is another example, which has recently been modified for flow through cracking clay soils by Morari and Knisel<sup>90</sup>. Also, the ADAPT model<sup>28</sup> was developed by combining algorithms from GLEAMS and the well known conceptual model DRAINMOD<sup>114,115</sup>. This hybrid water table management model considers macropore flow as a component of VSSM flow.

On the other hand, an example of models based on the FE scheme is the one developed by Antonopoulos and Papazafiriou<sup>7</sup>. They used the Galerkin FE method, the most common FE scheme used in soil hydrology, to solve one-dimensional, vertical transient flow of water and mass transport of conservative solutes in variably saturated media. Another example is the SAWAH model<sup>140</sup>, which simulates simultaneously saturated and unsaturated flows in a soil profile, including the case where moving saturated horizons exist



above the water-table level. SAWAH operates with variable time-steps and uses implicit and explicit schemes for unsaturated and saturated flow respectively. Another FE method is boundary integral equation, also known as Boundary Element (BE), that lessens the dimensionality of the problem by one, and initially solves the problem on the boundary of its domain only. An interior solution can then be sought from the boundary solution. Taigbenu<sup>122</sup> and Montas et al.<sup>89</sup> have applied this method to solute transport and preferential flow problems respectively. Ju and Kung<sup>68</sup> have compared lumped mass with consistent mass, and linear elements with quadratic/cubic elements in FE VSSM models. For a time-dependent problem with a large and complex domain, they suggest the use of a lumped mass scheme with linear elements. They also concluded that in such a case the time step should not be constant.

In any case, some general problems face both FD and FE methods. Difficulties in estimation of the effective value of hydraulic conductivity ( $K(h)$ ), which significantly controls the model outputs, is one example of such general problems. Moreover, knowing the rightful spatial/temporal average values of  $K(h)$  in the discretized domain is important. Especially when soil-moisture differs sharply between two adjacent nodes or when rapid temporal changes happen. Admitting the importance of inter-node hydraulic conductivity calculation methods on numerical models, Li<sup>77</sup> recommended the use of a composite integration formula, where each increment is subdivided into a number of intervals, to gain the best results. Another general problem is the high computational cost, especially in 3D VSSM flow simulations. To reduce the computational cost, Huang et al.<sup>62</sup> established a new convergence criterion for the numerical solution of the "mixed based" VSSM governing PDE. They compared this with standard and mixed convergence criteria and found a considerable decrease in the computational cost; especially, when the initial soil conditions are very dry or when soil hydraulic characteristics were extremely

nonlinear. In fact, these are conditions where numerical solutions with standard or mixed convergence criteria fail to converge, become unstable, or only slowly convergent. The most important advantage of FE over FD schemes may be conceived as flexibility of the FE grid that can be adapted to irregularities of the external and internal boundaries of the flow domain. However, FD schemes may be preferred due to their better stability for VSSM flow problems, as found by Celia et al.<sup>19</sup>. A hybrid approach, crossed from FE and integrated FD, in VSSM modeling is 'control volume FE' as described by Patankar<sup>98</sup> and employed by Di Giammarco et al.<sup>37</sup>. Hence, the model is conservative at local scales, and capable of dealing with irregular and complex geometries.

Concurrent to modeling practices on VSSM flow, many researchers have tried to simulate VSSM flow components in separate models or with an emphasis on a single component. Some instances of such components and research works are listed here: infiltration (Basha<sup>13</sup>, Castelli<sup>18</sup>, Cho et al.<sup>25</sup>, and Chu<sup>26</sup>); actual evaporation from bare soil and/or actual transpiration (Droogers<sup>40</sup>, Yakirevich<sup>143</sup>, and Yamanaka et al.<sup>145</sup>); preferential flow (DiCarlo et al.<sup>36</sup>, Gerke and van Genuchten<sup>47</sup>, and Workman and Skaggs<sup>141</sup>); soil deformation and/or swelling (Chertkov and Ravina<sup>24</sup>, Garnier et al.<sup>46</sup>, and Tariq and Durnford<sup>125</sup>); redistribution (Mitchell and Mayer<sup>86</sup>, and Ogden and Saghafian<sup>93</sup>); and hysteresis (Hopmans et al.<sup>61</sup>, and van Dam et al.<sup>131</sup>). Effective parameters and data uncertainty were two important issues in VSSM flow research works during these years. Both issues aimed to provide more realistic estimates of VSSM flow parameters that explain the real world situations to the model in a better way. Among researches of these kind use of so called "inverse methods" (e.g., Hughson and Yeh<sup>63</sup>, Lehmann and Ackerer<sup>73</sup>, and Takeshita and Kohno<sup>123</sup>) and "statistical and stochastic measures" (e.g., Mishra and Parker<sup>85</sup>, and Zacharias and Heatwole<sup>152</sup>) were dominant. Wildenschild and Jensen<sup>137</sup> have studied and compared different effective parameter estimation methods for soil hydraulic

characteristics. They concluded that none of the practical methods performed well, but among other field feasible methods, stochastic methods were found more reliable.

Soil Hydraulic Characteristic (SHC) functions are hydraulic conductivity function and soil-water retention function. Analytical equations for SHC have improved to become more accurate and/or general. Work by Assouline et al.<sup>8</sup>, Green et al.<sup>50</sup>, Mace et al.<sup>81</sup>, Mallants et al.<sup>83</sup>, Mohanty et al.<sup>87</sup>, and Tzimopoulos and Sakellariou-Makrantonaki<sup>130</sup> are instances in this research category. Leong and Rahardjo<sup>76</sup> reviewed and compared most popular soil-water retention equations. They found Fredlund-Xing<sup>44</sup> equations more favorable. Leij et al.<sup>74</sup>, also, reviewed SHC functions; however, they did not conclude upon a single method as the best. Some other noteworthy research works on SHC functions and the SHC parameters have been done by: Rawls et al.<sup>102</sup>, Shao and Horton<sup>108</sup>, Sidiropoulos and Yannopoulos<sup>110</sup>, and Simunek et al.<sup>112</sup>.

Knowledge of soil-plant relationships is essential in many AES simulation cases; therefore, some VSSM modelers have considered plants interactions with soil in their models. For example, knowing that root distribution affects soil-water flow and plant water uptake pattern<sup>21,70</sup> mechanisms of root growth and soil-water uptake have become modeling subjects. Jonse et al.<sup>67</sup> have proposed a conceptual approach to model main root growth properties. They have taken into account different soil factors affecting rooting. Clausnitzer and Hopmans<sup>29</sup> have developed a transient 3-D model of root growth and soil water flow, where root elongation of a single plant is simulated via translocation of the root apices in individual growth events as a function of current local soil conditions.

The surrounding environment is detached from simulation domain and replaced by boundary conditions (BC). Therefore proper setup of the BC has key importance in the modeling process. The soil surface, usually selected as the upper boundary, is the interface between soil and atmosphere; where infiltration

and evaporation or evapotranspiration takes place. From models that have been developed for the upper boundary interface processes, few examples are mentioned here. A conceptual infiltration model with redistribution, which was developed first by Smith et al.<sup>118</sup> was improved by Corradini et al.<sup>31</sup> to become faster and simpler. The model is an analytical approximation of a single ordinary differential equation, and is claimed to be fast and accurate enough for most hydrological applications. Wilson<sup>138</sup> has proposed a model for surface flux boundary, which is based on a system of equations for heat and mass transfer in the soil-atmosphere continuum. In contrast to Wilson's approach, most other models totally discretise the soil from the atmosphere, even though it is not the case in reality.

Generally, 1D models have been evolved via two paths; first, expanding by embracement of more processes; and second, reinforcing by inclusion of more details of VSSM flow realities. However, their application is logically restricted to the pedon scale. Examples of multi-dimensional (2D/3D) models, generally not as popular as 1D models, are discussed hereafter. More FE based models may be seen among these models. In contrast to their ability to simulate more complex cases, their serious disadvantage is high computation cost. FLAMINCO, a 3D model developed by Huyakorn et al.<sup>65</sup>, is based on the Galerkin FE scheme, that simulates water flow and migration of non-conservative contaminants in a variably saturated and anisotropic porous media. The required CPU time to solve an example of 3D transient flow (a sudden drop in the drain's water level) in a drained field (200m x 200m x 20m) discretised into 1200 finite elements and 1584 nodes, was 100 minutes on a VAX 11/750 minicomputer. A second example is LINKFLOW<sup>54,55</sup>, a quasi-3D saturated-unsaturated model based on FD, which was developed to simulate movement of soil water under a cropped field during various water table management practices. It is comprised of two main components: a one-dimensional unsaturated flow module, and MODFLOW<sup>80</sup> that functions as a 3D saturated flow

module. The model requires 60 hours to simulate a 60-day period on a 33 MHz 486 PC machine. Almost the same approach has been pursued by Yakirevich et al.<sup>144</sup> to develop the QUASI-3D model. In their first paper, implementation of the QUASI-2D model, they have reported their 2D model being several times faster than two well-known 2D models: the SUTRA model<sup>119,134</sup> and the 2DSOIL<sup>96</sup> model.

Some selective examples of multi-dimensional models are listed here; even though, no information on their computation cost were given. The model developed by Wu<sup>142</sup> is a complex numerical model to simulate 1-, 2- and 3D simultaneous transport of water, heat, and multi-component reactive chemicals in saturated-unsaturated soils. The model is based on the Galerkin FE method. No declaration has been stated about the required CPU time, but the author has mentioned that the model has been developed and tested on a 486DX2-66 Personal Computer under a LINUX operating system. Gregersen<sup>51</sup> developed the SIM2D model, a 2D VSSM flow model that is based on a FE (Galerkin) scheme for the time-independent part of the Richards' equation, while employing a fully implicit FD scheme to estimate time derivatives. The VS2DT model, a 2D-FD model by the U.S. Geological Survey, was developed to simulate the interactions between surface water and ground water. The model may be used to simulate river and groundwater interactions as well as transports between the root zone and groundwater<sup>20,56</sup>. Russo et al.<sup>104</sup> developed a 3D-FD model, intending to improve the knowledge of flow/transport through a 3D heterogeneous porous media at real field scale. The model is based on a 3D mixed form of Richards' equation solved by a modified Picard method<sup>19</sup>. Flow field hydraulic properties, assumed as statistically anisotropic random space functions, were generated stochastically.

There are more multi-dimensional models not listed here, but none of them are as popular as most 1D models. Theoretically, unsteady multi-dimensional numerical models have the ultimate capability of dealing with real world

temporal and spatial variabilities; however, some problems are practically encountered. In addition to laborious work needed to develop such models, the lengthy execution time for these models is a matter of concern for practical applications, especially whenever several runs are required. Moreover, 3D models require a great deal of input data. This means that the quality of the model results is greatly dependent on the quality of input data. In other words, if each input data carries a small error then the accumulated error might discredit the model results.

Most important factors affecting the input data quality may be addressed as follow. The first factor is the extension of point values to the surrounding areas. Although, the assumption associated with this extension (i.e. homogeneous field) is not true for most cases, but it also is not practically feasible to measure the characteristics of a field (real heterogeneous system) at any point. Secondly, temporal variabilities make point measurements even less factual. Finally, measured data intrinsically are associated with errors to a degree and some input data are only estimated values assessed upon point-measured data. The first and second factors are due to the heterogeneity/complexity of natural systems, which neither can be captured minutely nor removed. In fact, comprehensive simulation of AES and satisfactory result interpretation requires that heterogeneities of these systems to be taken into account. Therefore, highly accurate results may not be expected when deterministic models are used to simulate non-deterministic systems, as is the case for most of the numerical models discussed. Yet, having not achieved the “perfect model”, some researchers have started to look in totally different directions. They have been seeking for some other approximate methods, that need less or simpler input data and/or have less computational cost, to be employed instead of 3D numerical models, provided that the results accuracy remains the same. A brief review of their attempts is given in the next two parts.

### **Alternative Approaches**

Progress in computer science, applied mathematics, and numerical computation methods have helped and promoted the VSSM modeling practices. Most of the alternative models are inspired from those impressions such as fuzzy logic, artificial neuronet, expert systems, fractals, and parallel computing. Tim<sup>129</sup> discussed some such computer technologies in relation to hydrology and water quality modeling; and has foreseen the impact of these technologies on those models. The technologies examined were: user interfaces, virtual reality, animation, remote sensing, geographical information systems, global positioning system, knowledge base systems, and object oriented programming. In his opinion 'scale problems in models' and 'data collection techniques' need more considerations and improvements. He also recommended the incorporation of all, or at least most, of the above-mentioned components in a comprehensive decision support system. This is a definite challenge to researchers.

Bertuzzi and Bruckler<sup>14</sup> adopted the scaling method proposed by Warrick<sup>136</sup> to estimate field-scale SHC from point measured values. With the scaled-up SHC, Pedon-scale models may be used as a lumped model to simulate field-scale problems. The method needs improvements and more field experiments for its validation. Yet, lumped methods are obsolete if spatial information at a minor scale is required.

Fractal models, which describe self-similar hierarchical systems as new tools, are suitable models to describe soil structure, and therefore SHC. For instance, Chen<sup>22</sup> developed a conceptual capillary model based on fractals that generated conductivity curves ( $K(h)$ ) very close to the measured values. A good review on SHC fractal models is done by Gimenez et al.<sup>49</sup>. This novel approach faces lots of unanswered questions that need more research. How to merge saturated and unsaturated fractal models is one such a question. In fact, the total model (saturated-unsaturated) may require more than one fractal dimension for

different scaling regions. In other words, the geometrical interpretation for different soil moisture conditions may vary, as in dry soils SHC mainly could be determined by surface area, whereas near saturation SHC is primarily a function of pore structure<sup>32</sup>. Kravchenko and Zhang<sup>71</sup> pursued such an idea using two fractal dimensions for wet and dry parts of SHC. How to parameterize soil pores system is another question in this domain. A study of this kind was the fractal model of soil-water retention function with a randomly connected network, developed by Bird and Dexter<sup>15</sup>, that revealed the pore connectivity importance in addition to importance of pore size distribution. Fractal modeling approach for SHC estimation is still recruiting and needs more explorations and improvements in different ways.

Simons<sup>111</sup> tried to describe the soil matrix as a permeable pore structure via “pore tree” model. The model simulates the pore structure via tree-shape porous sub-systems that are randomly interconnected through common branches. The model may be seen as an alternate mathematical explanation of soil matrix, in comparison with fractals. Simons has expressed his future plan to improve the model to couple convective and small scale diffusive transport.

Portraying VSSM flow as a diffusion-convection wave process and simplifying vertical soil-water flow, Smith<sup>116</sup> approximated the VSSM flow via an analytical model based on kinematic wave. The idea has tempted some other researches to pursue this path to VSSM flow modeling. Some examples are: Germann<sup>48</sup> on macropore flow; Mdaghrialaoui and Germann<sup>84</sup> on macropore and diffusive flow; and Singh and Joseph<sup>113</sup> on VSSM flow with crop-roots uptake. It worth to be mentioned that short execution time, main advantage of analytical models, is counterbalanced with the fact that analytical models are only applicable to simplified cases that may be accepted as rough estimates of real situations.

Ewen<sup>42</sup> developed a novel VSSM flow model, named SAMP (subsystems and moving packets). The model is approximate and stochastic due to random



movements of soil-water packets within and between the flow-field cells. Ewen claimed that his model is capable of improving the realism of simulations, especially for non-equilibrium VSSM conditions. Vollmayr et al.<sup>133</sup> employed stochastic modeling via application of a 2D Monte Carlo technique, where particles hop between the sites of a square lattice that represents the soil matrix. The model suites for parallel computing purposes and its results were acceptable for a simple 2D problem. Future practices will reveal capabilities of both models.

Harter and Yeh<sup>53</sup> have proposed a numerical-stochastic model with high-resolution Monte Carlo simulations. They concluded that the stochastic unsaturated flow theory, despite its simplifications, captures many fundamental principles of VSSM flow. The hybrid stochastic model developed by Loll and Moldrup<sup>78</sup> is based on two steps; first, a deterministic model using stratified data to produce a deterministic response surface, and second, a stochastic model through a Monte Carlo method using the deterministic response surface to provide the total model response. The model was tested for a 1D case successfully. A major contribution is claimed to be the ability to provide a fast and time efficient way to analyze the sensitivity of the stochastic model response to different inputs. Recently, Tartakovsky et al.<sup>126</sup> has described a deterministic alternative to the Monte Carlo simulation, without any up scaling. They developed analytical non-local (integro-differential) conditional moment equations. This is for cases where the scaling parameter of pressure head is a random variable independent of location. It was assumed that hydraulic conductivity is an exponential function of pressure head. The results compare well with Monte Carlo results and coincide with theoretical analysis.

Another novel approach in VSSM flow modeling is based on fractals, as employed for SHC and mentioned above. Pachepsky and Timlin<sup>95</sup> have developed an equation for VSSM flow as in fractal medium that differs from Richards' equation in its diffusion coefficient, which is a function of both soil-

water content and pore connectivity. This novel approach still needs more research and exploration.

Boufadel et al.<sup>16</sup> proposed a novel dimensionless formulation for 2D-VSSM flow that provides a guideline for scaling and designing physical models. They employed Bayesian estimations to fit the model to experimental data and found that VSSM flow scaling requires conservation of the ratio between capillary and gravity forces. Satisfactory results have implied that the model deserves more attention. Bayesian framework has been employed also by Abbaspour et al.<sup>1</sup> in an inverse procedure for subsurface flow parameter estimation. Their method is potentially applicable to VSSM flow parameters as well. The procedure is called sequential, inasmuch as one more iteration can always be made to get a final estimation of parameters.

Another set of promising alternative methods, in VSSM flow modeling/parameter estimation, is the application of Artificial NeuroNets (ANN) and Fuzzy Systems (FS). To emphasize on these approaches they are reported in the next part of this review separately.

#### **Application of ANN and FS to VSSM Flow Modeling**

Need for a better model approach able to imitate the real world with its complexity, dynamism and non-linearity, has motivated AES modelers to investigate any novel simulation technique. ANN and FL, two new computational intelligence technologies have received increased attention from ASE modelers. Utilization of ANN and FL technologies is new in modeling of SHP. Reported applications are, yet, few but increasing and promising. One of the first studies of this kind was reported by Altendorf et al.<sup>4</sup>, who used ANN to predict soil moisture from soil temperature data. They preferred the use of ANN because of its “black box” (or regression type) nature, which leads to a minimum number of input parameters, in contrast to “mechanistical” approach.

Bardossy and Disse<sup>12</sup> developed two fuzzy rule-based models for infiltration. The models, which are based on Green-Ampt and Richards' equations, are mechanistical but non-numerical. The authors concluded that their model need less input parameters and run much faster in comparison to classical models, however, the model was very sensitive to rule consequences (i.e. fluxes), which were not easy to be tuned/calibrated. Later, Bardossy et al.<sup>11</sup> extended the idea to model VSSM 3D-flow via fuzzy rules. The model was much faster than classical models and the resulting accuracy was acceptable, besides less input parameters were needed. However, still the same problem persists: a difficulty establishing proper rule consequences. Moreover, the model is sensitive to the number and definition of the fuzzy sets.

Shukla et al.<sup>109</sup> trained an ANN to mimic the Boussinesq equation in prediction of water table level. In comparison to the numerical Boussinesq model the ANN model was much faster. This trail was pursued by Yang et al.<sup>146-149</sup> who have developed several ANN models for prediction of water table depths and/or drainage outflow. Yang et al. have also applied ANN to simulate soil temperature<sup>150</sup>, and to simulate pesticide concentrations in soil<sup>151</sup>. Sreekanth et al.<sup>120</sup> analyzed some of papers on ANN modeling of water table depth and investigated the importance of input parameters in such models. A general conclusion drawn from ANNs fast execution and their generalization abilities is that they can be employed as ideal models/tools for many AES real-time problems such as automated water table management systems<sup>146</sup> and precision farming<sup>41</sup>.

A novel approach, suggested by Davary et al.<sup>34,35</sup> applies Artificial NeuroNet (ANN) and Fuzzy Inference System (FIS) to VSSM problems. The method helps to speed-up model execution as well as to facilitate input data preparation in two ways: via usage of soft data along with hard data; and via minimization of

number of input variables. The approach seems promising in speeding-up 2- and 3-dimensional VSSM models.

Pachepsky et al. (1996) developed an ANN model for soil-water retention relationships from easily measurable data. Concurrently, Tamari et al.<sup>124</sup> and Schaap and Bouten<sup>106</sup>, worked on the same subject. All three, studied and compared ANN with regression models and found the ANN models superior and more favorable. In fact ANN models has been replacing regression pedo-transfer functions in different VSSM domains due to their flexibility. For example, Schaap et al.<sup>105</sup> developed alternative ANN models, each with a different number of independent variables, to estimate soil-water retention and unsaturated hydraulic conductivity. They found ANN based functions performance superior to existing pedotransfer functions in two ways: enhanced accuracy, and availability of alternative functions for cases with different numbers of independent/input parameters. However, compared to regression equations, one disadvantage of ANN models is that the mathematical formulation does not symbolize any meaningful/physical relationship between inputs and outputs.

Acknowledging uncertainty of soil/aquifer parameters and to avoid expensive yet inadequate field parameter evaluations, Chen and Kao<sup>23</sup> adopted fuzzy variables within a geographical information system to generate parameter needs for groundwater pollution potentiality assessments. Same approach may be adopted to provide parameters needed for 2D/3D VSSM flow modeling based on easily measurable soil physical characteristics (soft/hard). Perret et al.<sup>99</sup> defined input variables as “fuzzy variables” to incorporate the uncertainty of these variables (namely: saturated hydraulic conductivity, drainage coefficient, and depth to an impermeable layer) into the drainage design process to find the mid-span water-table depth. The authors claim their model is considerably simpler than fully stochastic methods. Schulz and Huwe<sup>107</sup>, following a similar

logic, have assumed VSSM flow parameters (namely: saturated hydraulic conductivity, upper boundary water flux, and Gardener's coefficient for unsaturated hydraulic conductivity) as fuzzy variables and solved the 1D steady state VSSM flow. They compared fuzzy with stochastic approaches and concluded the fuzzy one as a very flexible tool for expression of model parameter vagueness or for introduction of soft data<sup>\*</sup> or linguistic parameters to the model. Almost in the same direction, Freissinet et al.<sup>45</sup> explained a fuzzy-logic-based approach to assess imprecision. Their method is to compute the output of a deterministic VSSM model as "mean response", then to estimate the imprecision range of the mean value via fuzzy computations using fuzzy variables. They described their method as a simple and flexible tool for risk analysis studies. Overall, employing fuzzy variables and fuzzy mathematics has brought into the opportunity to use soft data and has facilitated the inclusion of uncertainty for VSSM parameters.

In the quest for the "perfect model" numerous SHP computer simulation models have been developed, many of those reviewed in this paper, during last decades. To drive a single conclusion from these vast efforts and diverse achievements seems almost impossible. Then, in order to comprehend the wide spectrum of SHP models, a worthwhile sum-up is to classify these models into few categories, as is presented in the next part of this paper. This facilitates comparison of models and helps to drive an inclusive conclusion.

### **GENERAL CLASSIFICATION OF SHP MODELS**

Before getting into classification of the models few points have to be clarified. Firstly, models may be classified as single-process versus multi-process. SHP computer simulation models, mostly, are multi-process models. Such multi-process models include different parts or processes, usually referred to as sub-

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<sup>\*</sup> "Soft" data is qualitative information, in contrast to "Hard" data or quantitative information.

models, which may be modeled technically in a different way. Therefore, most often, classification of multi-process models is impossible. However, a single-process model or any sub-model can be categorized in a certain class. Secondly, models may be classified from different points of views. In fact, different systems of classifications have been suggested and inaugurated; most of those are not contradictory to each other, but complementary. Thirdly and the last, to consider any model in a certain class a minimum information is required, and to compare models to each other even more information, especially on model performance, is needed. Unfortunately, most of the model reports do not provide this information, while they present supportive information on their pros. It seems that a kind of “model report guideline” would be very beneficial if followed by authors of papers on newly developed or enhanced models. The information offered in such papers should, for instance, include facts on: the model computation cost, the algorithm employed, and the platform used. Now that the initiative points are addressed, the proposed ‘model classification’ is described next.

At the root level, models may be classified as “*physical*”, including “*analog*” and “*replica*” models, versus “*non-physical*” models. In the latter case, also called “*abstract*” or “*conceptual*” models, the modeled relationship may be presented via different means such as equations, graphs, databases or tables, rules, and linguistic knowledge-bases. Regarding the point of view adopted, *non-physical* computer simulation models in turn, as discussed below, may be categorized in different ways.

First way to classify non-physical models is to consider them in two sub-classes: “*black-box*” and “*white-box*”. Between these two extremity there lay “*gray-box*” models which are not purely white. Models that are originated from phenomenal explanations are admitted as *white-* or *gray-box* models. Then, most of SHP *non-physical* models are of this kind, and *black-box* models are rare. However, *black-box*

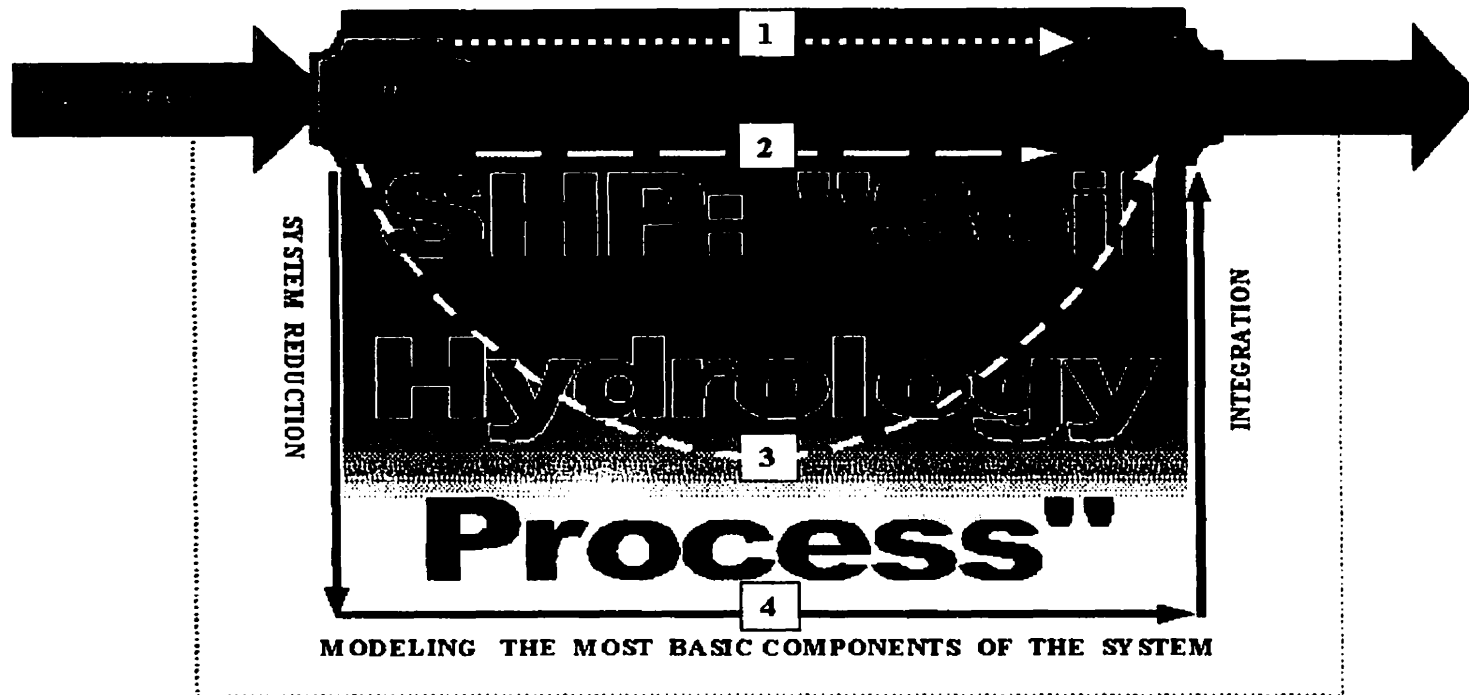
models are favorable for simulation of very complex phenomena that are not yet, even partially, comprehend or explained. They model the relationship between inputs and outputs blindly, i.e. the model does not explain the real physical link between inputs and outputs, and is not informative about the internal processes of the prototype. Mostly, regression and ANN techniques have been employed to define *black-box* models. If neither model formulation nor its parameters are known beforehand and they are expected to be determined from data then the model is a *pure black-box* model. Rules or linguistic knowledge-bases may also be used to define a *black box* model.

From a second angle of view, *non-physical* models may be categorized in sub-classes as “*mathematical*” versus “*non-mathematical*”. The fact that computer technology is based on binary digit system has led the modelers to deal with the continuous processes in a discrete manner. Moreover, soft data or qualitative variables had to be expressed as hard data or quantitatively (i.e., translated into numbers). It was not easy for model users to adopt these artificial views. Not exceptions, SHP computer simulation models, too, have been based on *mathematical* expressions that only accept numbers as their inputs. In many cases these models have also been based on *numerically* expressed models that discretize the model domain (space/time). Along with the innovations in computer technology (such as fuzzy logic, expert systems, parallel computing, and fuzzy based processors) gradually new computer simulation models based on *non-mathematical* expressions are emerging. On the other hand, *mathematical* models have been evolving to become capable of handling the real world uncertainty through utilization of different tools such as Monte-Carlo simulation, Bayesian estimation, and fuzzy mathematics. These breakthroughs have bestowed upon computer simulation models the ability to, somewhat, handle soft data as inputs and/or outputs. Sub-classes of the *mathematical* models are “*analytical*” and “*numerical*” models.

Thirdly, *non-physical* models may be grouped into “*deterministic*” and “*non-deterministic*” models. *Deterministic* models are founded on the premise that an almost accurate anticipation of a SHP response, due to any certain excitation, is achievable. The conflict between *deterministic* approach and soil heterogeneity has restricted the application of *deterministic* models mostly to very small-scale problems. To overcome the scale barrier, deterministic models have evolved via adoption of the “effective parameter” concept. The concept is to estimate lumped parameters from a heterogeneous domain in a way to assure the proper model output, possibly using inverse methods. But, as the domain gets larger and/or more heterogeneous and also as the share of *deterministic* sources decreases in the domain heterogeneity, the model inputs become more uncertain, which leads to a more *non-deterministic* model. Hence, due to the scale dependency categorization of models is somewhat confusing for the two classes. The traditional *non-deterministic* modeling approach, *stochastic* modeling, which has been in practice during the last three decades, resolves the scale barrier statistically. Alternatively, a novel *non-deterministic* approach employs *fuzzy* variables as inputs to model.

The last view, which is very similar to the first one, classifies SHP models into “*empirical*” and “*mechanistic*” sub-classes. The crudest *empirical* models are *pure black-box* models. Other *empirical* models consider some physical aspects of the prototype to define the model formulation, at least partially. These models are still dependent on the data, mostly for the determination of model parameters. Inasmuch as the *empirical* models are in debt of data for their existence they are also called “*data driven*” models. As much as a model considers physics of the process modeled, it becomes more independent of data and more *mechanistic*. In contrast to a “*pure black box*” model, the other extreme end of this classification is a “*fully mechanistic*” or “*pure white box*” model. A “*fully mechanistic*” model breaks down the main process, reducing it repeatedly to sub-processes. Eventually, the





**Figure 2.1.** Graphical presentation of SHP models classification.

- The fine dashed box represents any "SHP system".
- Dotted line labeled 1: "pure black box" model.
- Dashed line labeled 2: "empirical" model.
- Dashed line labeled 3: "mechanistic" model.
- Solid lines labeled 4: "pure mechanistic" model.

most basic components of the system are revealed, then it executes the modeling task, followed with an integration of the results to get back to the main process level. Figure (2.1) graphically explains some of classification aspects discussed here. It is obvious that no distinctive partition exists between *empirical* and *mechanistic* models.

Any single process model can be classified according to all the views mentioned above simultaneously. For example DRAINMOD<sup>114,115</sup> developed by Skaggs, is an original *conceptual* model that employs water balance analytical equation in a soil profile confined between the soil surface and a shallow water table. The model executes quite fast on a PC, but has limitations: it does not provide soil moisture content data through the soil profile, and its concept has been developed for only one-dimensional vertical flow. DRAINMOD, then, is classified as a *conceptual, white-box, deterministic, and analytical-mathematical* model. It may be considered at the same time as *mechanistic* (not *fully mechanistic*) too.

Models may, also, be categorized under some other groupings. For instance: *discrete* versus *continuous* models (regarding the events duration and sequence), *steady* versus *unsteady* or *transient* models (considering dynamics of the model), *one-* or *two-* or *three-dimensional* (with respect to the model spatial extent), and *research-* versus *practice-oriented* (due to the model utilization mode).

## CONCLUSIONS

Periodical comprehensive technical reviews and summing-ups on soil hydrology models, such as one published by Feddes et al.<sup>43</sup>, are very useful and necessary for SHP modelers and model users. In the lack of such review papers, present paper has tried to present a brief review; however, it tends to emphasize on alternative modeling approaches.

Reviewed models in this paper show that existing SHP models mostly can be classified as *deterministic-mathematical(-numerical)-mechanistic*. However, in recent years, alternative models have gradually become a visible trend in SHP modeling. Along this trend number of *non-deterministic*, and *non-numerical* SHP models has been growing due to new opportunities provided. For example, use of fuzzy variables in VSSM modeling has opened a way to employ linguistic variables. Also, use of ANN models has facilitated modeling of highly complex and non-linear relationships with reasonable error, even when data is uncertain/noisy.

ANN models are data driven type models where in order to obtain the best match between the historical data set and the simulated data set, model parameters (weights) has to be adjusted while minimizing the error. Mathematicians have shown that multi-layer feed forward ANNs have the powerful capability of being universal function approximators<sup>57</sup>; hence, they are best suited for modeling complex relations<sup>82</sup>. Particularly, ANN models are very useful when data are vague. These specifications are pivotal to the modeling of SHP, especially the complex VSSM flow problem, with uncertain and noisy data. FIS, in the other hand, brings the possibility of soft data acceptance as inputs and also provides a simple method to deal with the non-determinism of the VSSM flow parameters.

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## **CONNECTING TEXT: CHAPTERS TWO & THREE**

Chapter two presented a review on SHP simulation models with an emphasis on recent novel approaches. From this the reader is exposed to the general evolution of SHP models and the problems with customary types of models. At the end of this chapter, a novel modeling approach is mentioned that is based on ANN and FIS utilization. Chapter three introduces this novel approach developed in the course of this study. It also contains an introduction to ANN and FIS and how they have been employed in VSSM redistribution modeling. Chapter three presents the first 1D ANN-based VSSM redistribution model. This model was developed to test the ANN-FIS based approach. ANN training results and the 1D model test results (against the SWAP93) are given at the end of chapter three.

If VSSM flow is to be modeled numerically, then the Richards' equation is employed. This equation is derived from the 'continuity' equation and 'Darcy-Buckingham' equations. Therefore Richards' equation is subject to the assumptions of the source equations. On the other hand, the ANN-FIS based model, introduced in the next paper, is not based upon equations but learns from data, hence no assumptions need to be considered. This novel approach has the potential of more closely modeling reality. Also, phenomenon such as preferential flow may be incorporated directly into the model if the records (observed data) contain the relevant information.

## **CHAPTER THREE: A NON-NUMERICAL 1D MODEL**

**ABSTRACT:** This chapter explains a novel approach to variably saturated soil moisture (VSSM) movement modeling. In contrast to the conventional numerical approach, based on solution of Richards' equation, the novel method employs artificial neuronet (ANN) and fuzzy inference system (FIS) techniques to solve the flow between two adjacent soil compartments. This chapter also presents a VSSM one-dimensional transient flow model as an example of the novel approach. The Darcy-Buckingham equation for steady VSSM flow was employed to generate training data for the ANN. The model was then tested against SWAP93. A good match with the numerical model output was found. Maximum error was less than 8%, which in comparison to the variance usually associated with the input parameters, seems quite acceptable.

### **INTRODUCTION**

Variably Saturated Soil Moisture (VSSM) flow models are powerful tools, which can serve in planning, designing, and managing irrigation/drainage or any other soil-water related process. For instance, these models are often used for simulation of project alternative scenarios to give more insight into likely benefits and drawbacks. If the spatial/temporal environmental impacts of the alternative project settings converge, then selection of the safer and more environmentally friendly scenario is possible.

Richards' equation, the governing partial differential equation (pde) for unsteady-variably saturated flow in an anisotropic-heterogeneous multidimensional porous media, has been commonly used as the kernel for VSSM flow computer simulation models. The unsaturated hydraulic conductivity function, a coefficient in the governing pde, is rarely measured, but is usually estimated and used by the model as a typical regional value. At best,

the function is estimated from point-measured values of “saturated hydraulic conductivity” and “a soil moisture retention function”. Even the latter one is usually measured from disturbed soil samples in the laboratory. Solution of Richards' pde is associated with many programming efforts, and often has high computation costs. Results, however, are merged in great detail with uncertainty due to temporal/spatial diversities, intrinsic to the VSSM input parameters. These problems are evident, to a greater degree, for more complex models such as three-dimensional (3-D) models. Therefore, results of such models can only be regarded as rough approximations of reality<sup>1</sup>.

A novel approach, based on application of Artificial Neuro-Net (ANN) and Fuzzy Inference System (FIS) techniques, was suggested by Davary et al.<sup>4</sup> that seems persuasive in resolving at least some of the above mentioned problems. This paper introduces the novel approach in detail, by presenting a one-dimensional VSSM flow model named ANN-FIS-1D that lowers programming efforts. For multi-dimensional cases it is also expected to lessen the computation cost, as well as to facilitate the preparation of inputs, via acceptance of 'soft' data and a decrease in the number of inputs. This paper also presents a simple 1-D transient ANN-FIS-1D model. The paper starts with a brief review of foundation concepts of ANN and FIS techniques. Then, development of the sample model and its sub-modules, including the ANN and the FIS, is explicated. Finally, results of the model and that of SWAP93<sup>15</sup> are compared.

## **FOUNDATION CONCEPTS**

The main idea is based on the usage of ANN, which is known to have a powerful capability of being a universal function approximator<sup>7,8</sup>, used in place of Richards' equation as the heart of a model. Richards' equation was originally derived from “Darcy-Buckingham” and “continuity” equations. Therefore, it is subject to the Darcy equation limitations. Moreover, Richards' equation does not count for other forms of flow other than Darcian flow, such as preferential flow

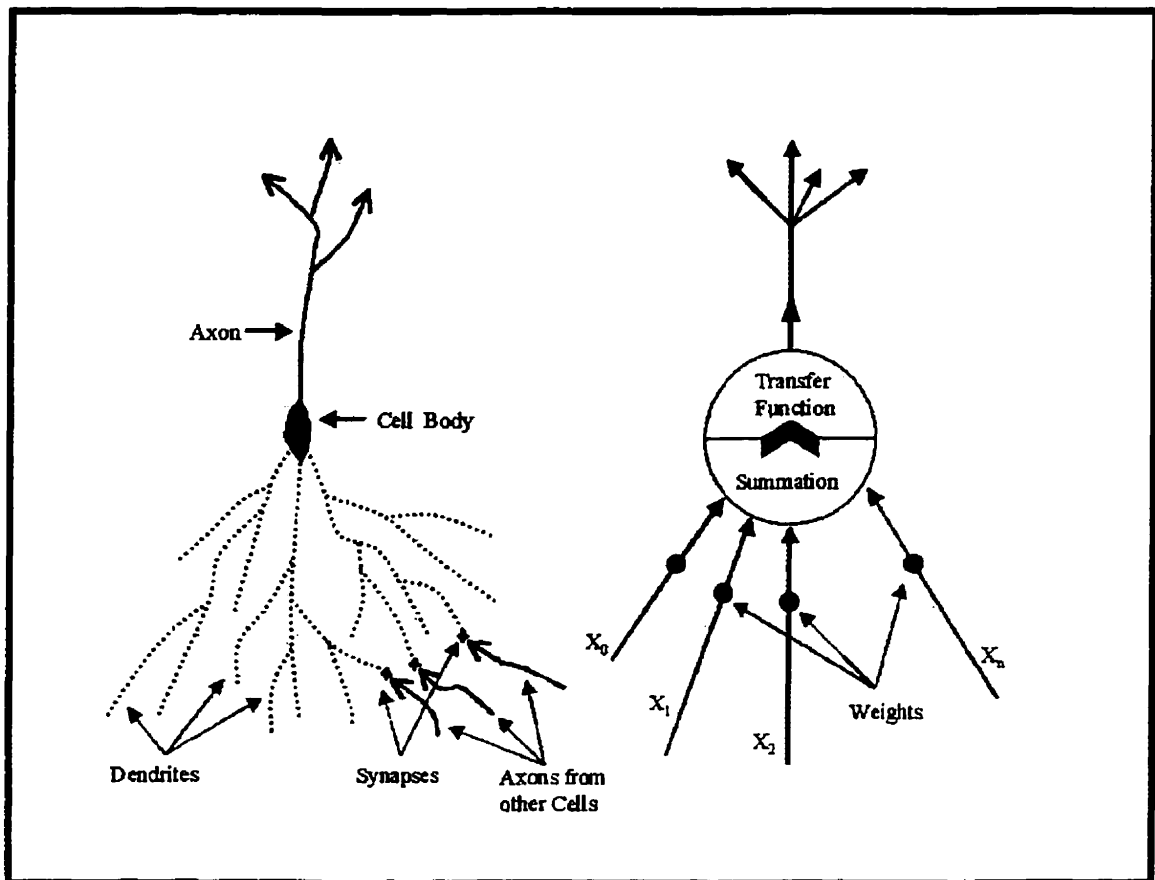


Figure 3.1. Basic structure of a Neuron and the diagram of a neurode or processing element (PE).



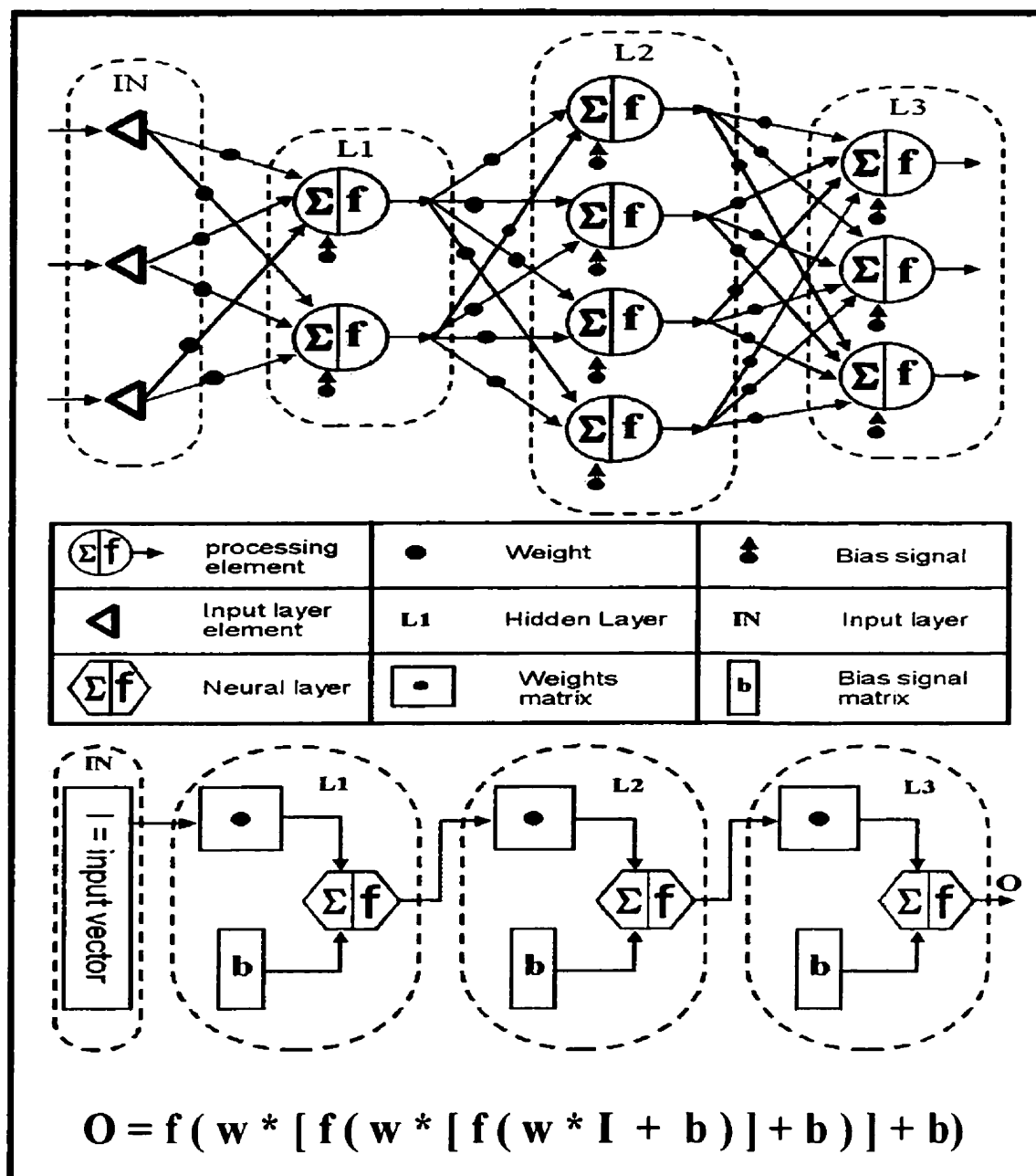
and salinity induced flow. Traditionally, VSSM flow numerical models, based on Richards' equation, utilize other equations for these additional circumstances. However, the ANN model can overcome such limitations, if trained with a comprehensive set of field data including information on macropores, salinity, ... etc.

To minimize the ANN approximation error on the highly non-linear VSSM flow, usage of multiple overlapped ANN ranges was adopted. Consequently, the need for several ANNs, and integration of the outputs brings FIS into the framework. The next two sub-sections briefly introduce these ANN and FIS techniques.

### **Artificial Neural Networks**

Artificial Neural Networks (ANN) are brain-like information processing systems. They are composed of several simple "Processing Elements" (PE) called "neurodes", which are models of human nervous system cells, "neurons"<sup>2</sup>. Analogous to a brain, an ANN is a highly parallel, intensively interconnected processing system<sup>12</sup>. The resemblance of the model (neurode) to the prototype (neuron) is obvious in Figure (3.1).

ANN "learns" from examples (sets of conjugated input-output data). The process through which ANN captures the relationship between input and output vectors via its weights ( $\equiv$  parameters) as well as its structural architecture ( $\equiv$  formulation) is called training. Figure (3.2) demonstrates a multi-layer feed forward ANN. The expanded layout, at the top, shows all neurodes and their connections. In the middle the same network is shown in a more compact fashion using matrix notation. Mathematical expression of the same ANN is presented at the bottom. Usually subscript notation is used for labeling weights, for instance  $W_{L(i,j)}$ , where  $L$  is the layer index,  $i$  is the current layer neurode index, and  $j$  is the previous layer neurode index. Structural components are number of inputs, outputs,



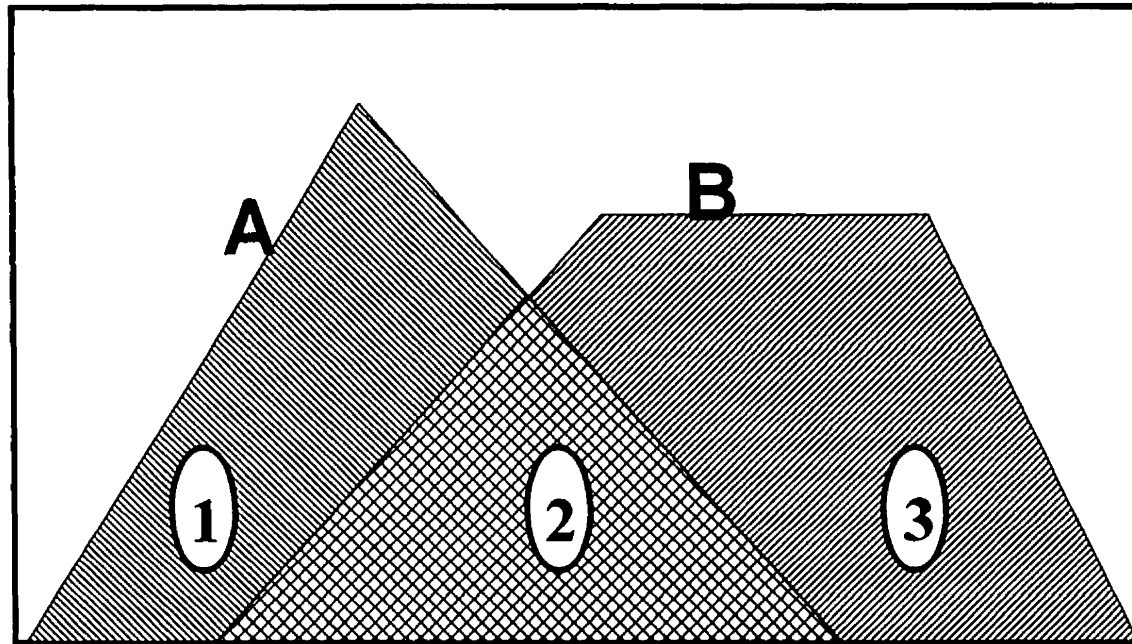
**Figure 3.2.** Expanded and matrix-form schematic diagrams, and mathematical expression for a multi-layer feed-forward ANN.

layers, and neurodes of the ANN, and also the neurodes architecture (i.e. arrangement and connection layout).

The fact that ANN learns by means of training offers a powerful alternative to programming. Training is accomplished through weight adjustment, while it seeks the minimum network error (the difference between the desired output and the network estimate). Training is an iterative process composed of two main steps in each iteration. First, some input vectors are introduced to the network to estimate relevant output vectors. This is called 'feed forward' activity. Then, comparison of estimated and desired output vectors produces error signals, which are directed back to the ANN for modification of the weights. This is called 'back propagation' activity. There are different methods used for modification of the network weights, called learning rules or learning algorithms. The 'delta rule' is one popular learning rule. Basically, it is a 'least sum of squares of errors' (LSE) method, and is usually improved by a momentum term. The momentum term is added to give the algorithm a breakout chance, if found to be trapped in a local minima instead of the global minima.

### **Fuzzy Inference System**

Complexity (non-linear and chaotic behavior) and dynamics (spatial and temporal changes) of real world systems can not be easily captured via observation and may not be precisely explained by point-wise collected data (in time and space). Therefore, data uncertainty is unavoidable. The degree of fuzziness or vagueness in the uncertain data depends on the degree of system complexity, acuteness of system heterogeneity, precision of data measurement method, and intensity of data collection points. In general, as stated by Zadeh<sup>17</sup>: "As complexity rises, precise statements loose meaning and meaningful statements loose precision." To consider this vagueness in the course of reasoning and calculations Zadeh<sup>16</sup> introduced 'fuzzy logic'. An FIS is a combination of rules with fuzzy premises and/or consequences that employs



**Figure 3.3.** Fuzzy sets (A & B) and classic logical operators.

$$A \text{ .AND. } B = 2$$

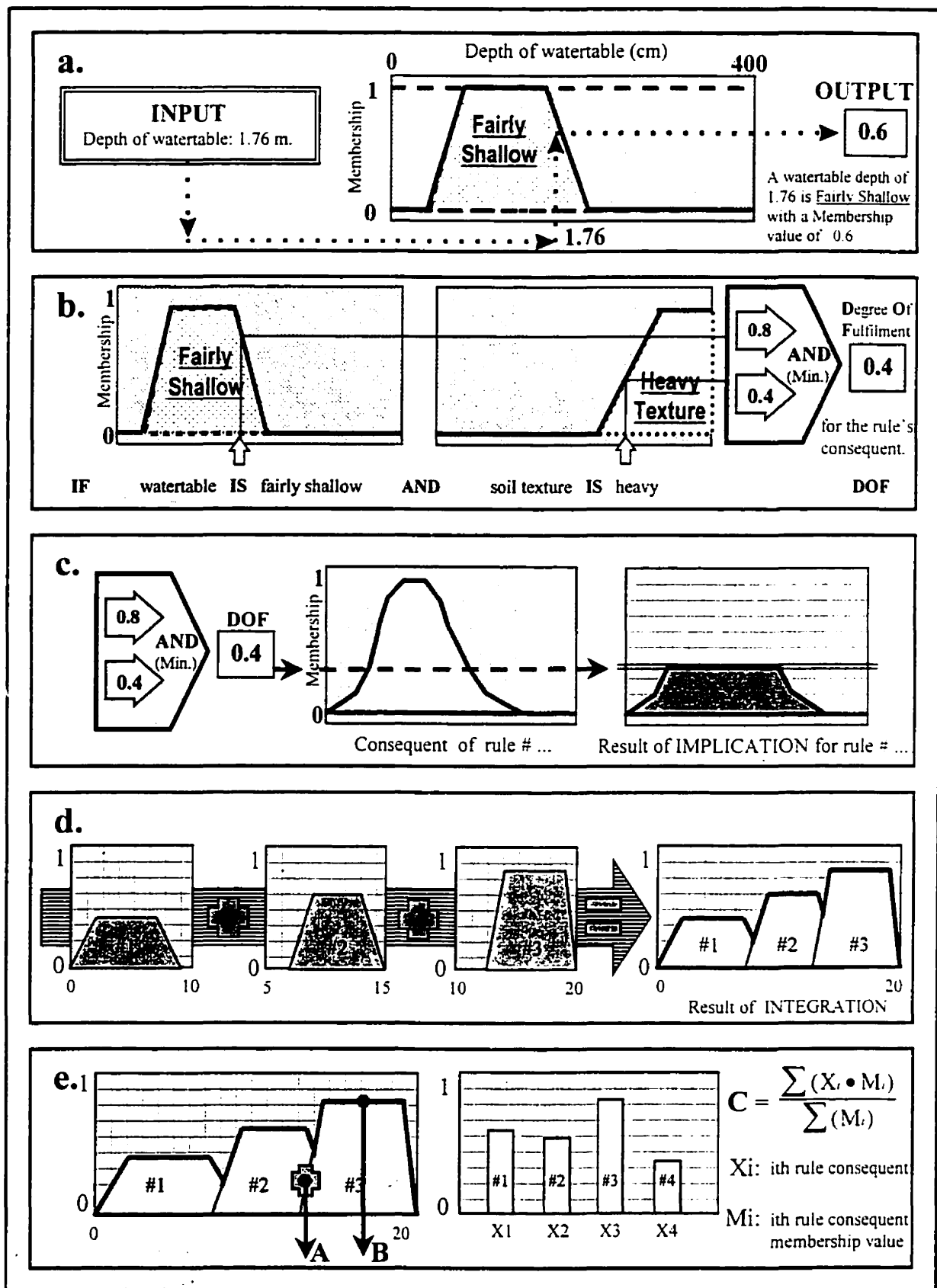
$$A \text{ .OR. } B = 1 + 2 + 3$$

$$\text{.NOT. } A = 3$$

fuzzy logic for its inference task. Elements and steps involved in a FIS are introduced below.

A fuzzy set is a set that can contain elements with partial degrees of membership<sup>6</sup> meaning that it has graded (not clearly defined) boundaries. This is in contrast to ordinary sets with rigid/crisp memberships (only 0 or 1). A membership function, for a given fuzzy set, is the function that assigns appropriate membership degrees (0 to 1) to each point in the universe of discourse. Classic logical operators and their operations on fuzzy sets are presented in Figure (3.3). Fuzzy sets, membership functions, and logical operators are elements of 'if-then' rules that in turn are main components of an FIS. Stages of an inference process (Figure 3.4) may be described in five steps<sup>1,9,13</sup> as follow:

- a. Fuzzification of the input(s): to resolve all fuzzy statements in the antecedent to a degree of membership ( 0 to 1 ).
- b. Application of fuzzy operator(s): to apply fuzzy logic operators to components of the antecedent, and resolve the antecedent to a single number ( 0 to 1 ), this is the degree of fulfillment (DOF) for that rule.
- c. Implication: to fire the rules with non-zero DOF and find the consequences or outputs of these rules.
- d. Aggregation of the rules outputs: to unify or integrate all outputs together to make a combined output for the FIS.
- e. Defuzzification of the output: in most cases a fuzzy output is not a suitable output format. Therefore, this step transforms the aggregated output, which is fuzzy, to a single crisp value. There are different defuzzification methods available such as: centroid, middle of maximum, and Sugeno.



**Figure 3.4.** Schematic Fuzzy Inference System with three methods of defuzzification (A: Centroid, B: Maximum, and C: Sugeno)

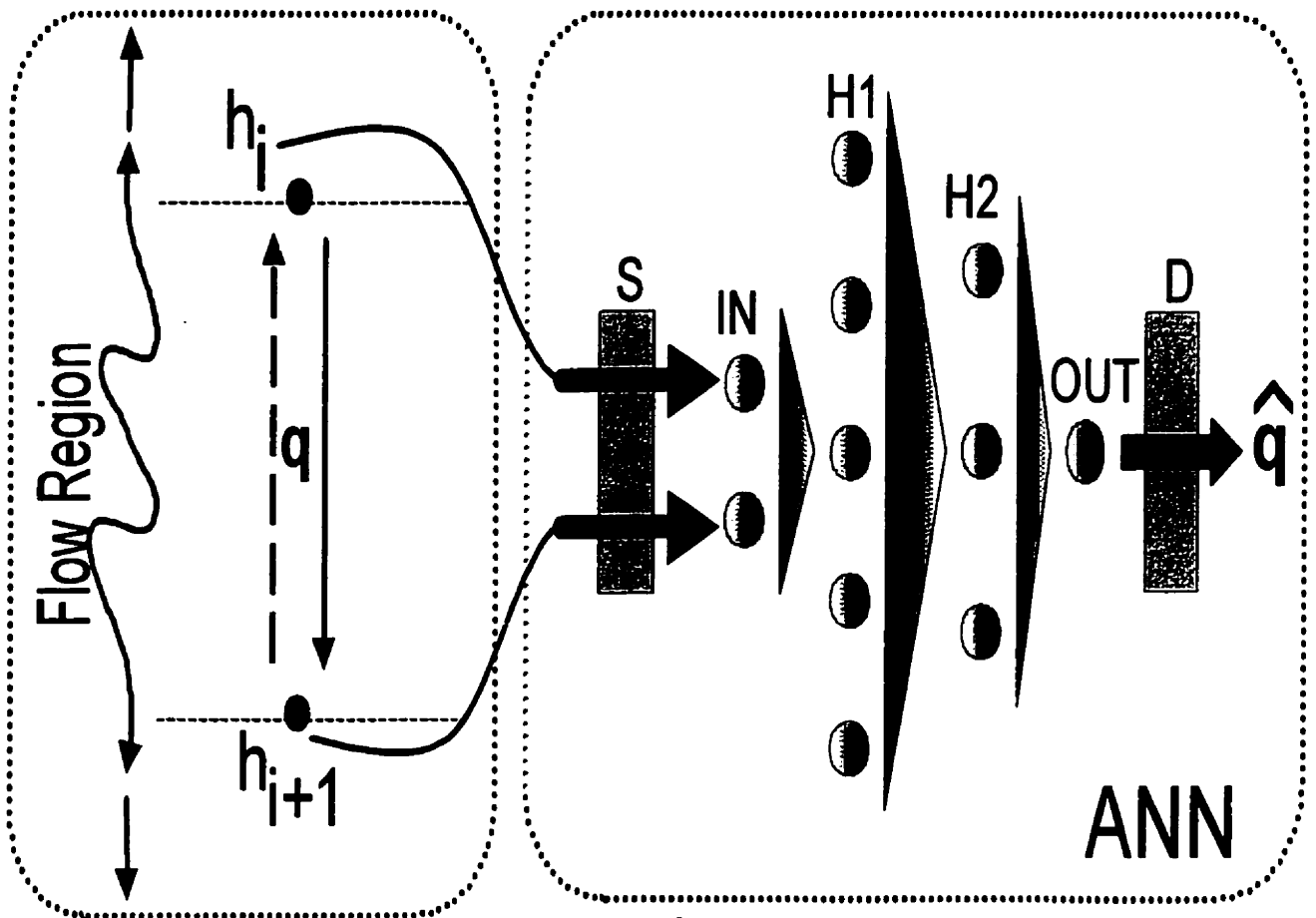
## **MODEL DEVELOPMENT**

To demonstrate the novel VSSM flow modeling approach used in this paper, a sample model was developed. This was done in three main steps, namely: development of the ANN module, development of the FIS module, and integration of these modules into the main model which simulates the VSSM flow through time (simulation period) and space (flow region). Then, the performance of the model for a simple soil-moisture redistribution case has been tested and compared against the results of SWAP93 model, an off-spring version of the well-known SWATRE model<sup>3,5</sup>. While the results and discussions are presented in a following section, the subsequent section provides details on the different model development stages.

### **The ANN Module**

Original soil data, taken from a table in the DRAINMOD reference report<sup>14</sup>, contains: 'soil-water content' associated with relevant 'soil-water head' and 'unsaturated hydraulic conductivity' values. In order to provide enough tabular points for data generation, this table was extended from 42 to 153 data rows, using 'CurveExpert'<sup>10</sup>, a curve fitting software.

The ANN structure (Figure 3.5) was selected, via trial and error, to have two hidden layers with five and three neurodes in the first and second layer, two inputs (i.e., head values of two adjacent nodes in the soil) and one output (i.e., steady flux between the two nodes). Accordingly, all records in the ANN training data must have three values (two heads and a flux). A small FORTRAN program based on the Darcy-Buckingham equation, with an arbitrary fixed nodal distance equal to five centimeters, was developed to generate 23,562 records to be used as ANN training data. In this study, 'Microsoft PowerStation FORTRAN compiler - V1.0', was used for this and other programming purposes. The ANN module was trained by 'Neural Works Professional II/Plus - V5.23', software.



$$q = k(h) * \left( \frac{dh}{dz} - 1 \right) \approx \hat{q}$$

**S : Scaling**

**D : De-scaling**

**IN : Input Layer**

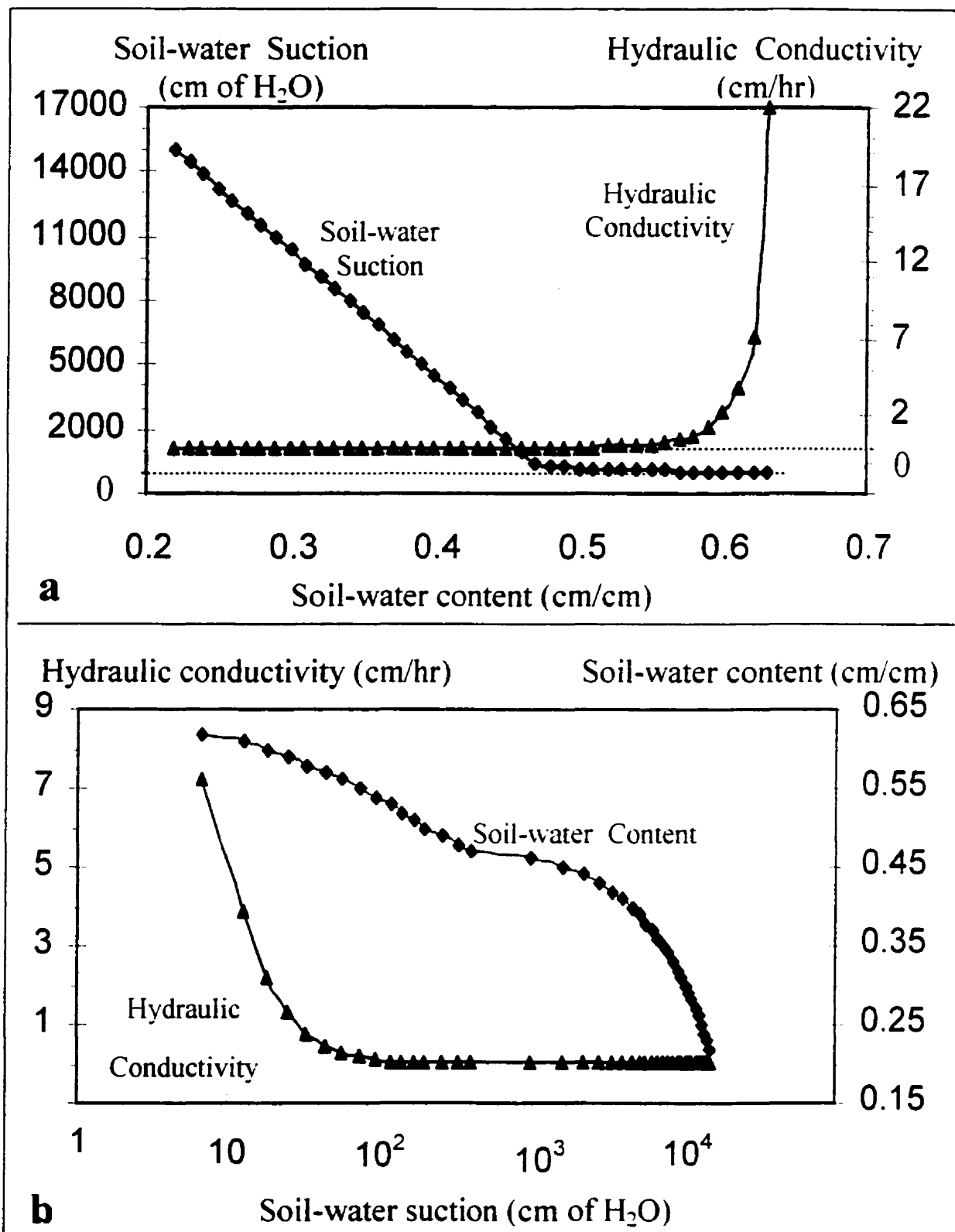
**OUT : Output Layer**

**H1 : Hidden Layer 1**

**H2 : Hidden Layer 2**

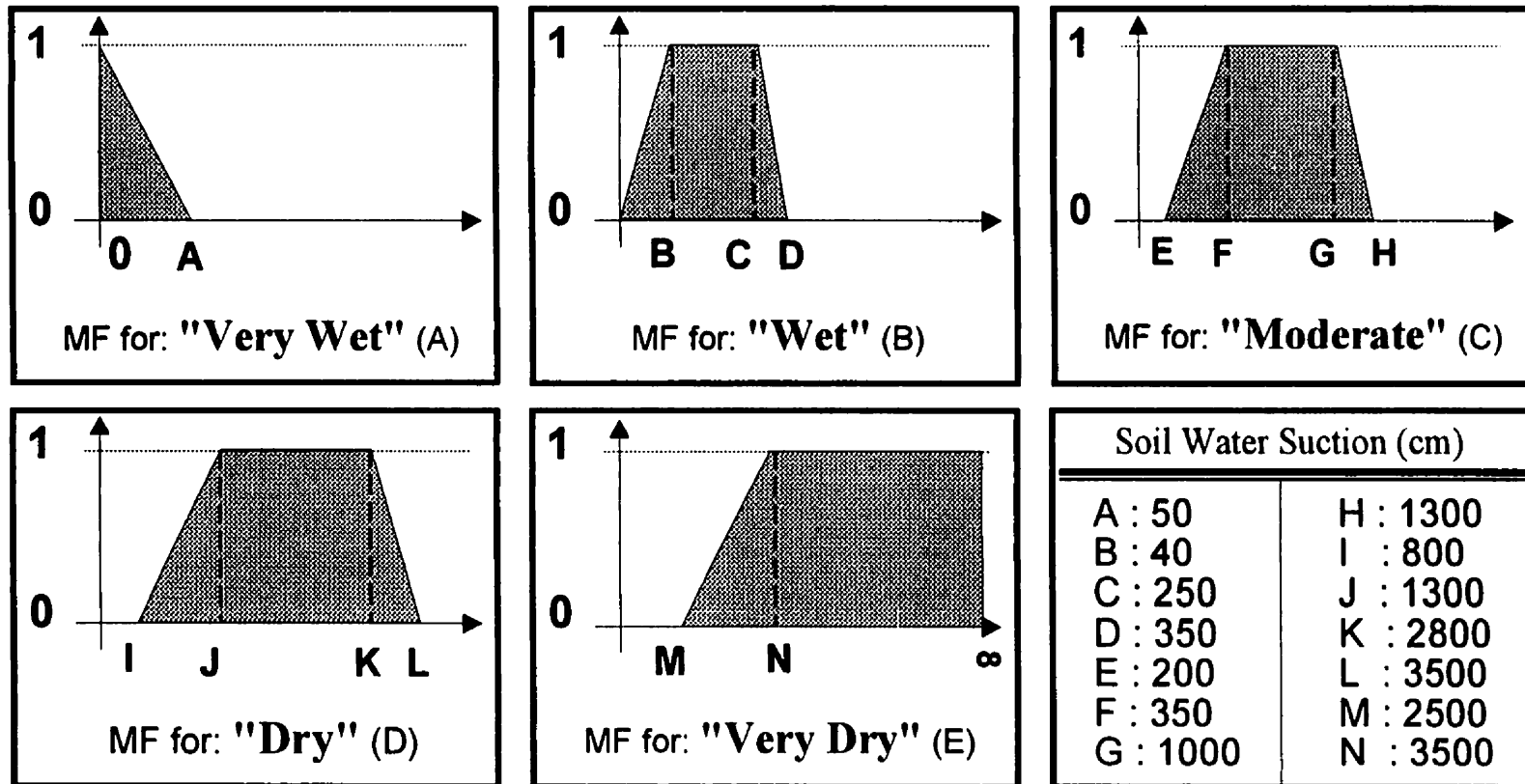
**Figure 3.5.** The ANN kernel in the model estimates fluxes between any two adjacent nodes within the flow region.





**Figure 3.6.** The hydrodynamic functions used in this study

- a) The graph shows the large difference between slope variations of the two functions.
- b) The logarithmic plots of the functions reveal inflection points, used to setup the fuzzy sets.



**Figure 3.7.** Fuzzy sets for soil-water suction, with membership on the vertical axis and soil-water suction on the horizontal axis.

Initially, training was done for the whole range of fluxes (-0.00020278 to 0.00014167 m/s, negative sign denotes downward flux). However, due to unsatisfactory results it was decided to divide the flow rates into sub-classes in order to decrease nonlinearity and provide a better chance for ANN training. Taking inflection points of the soil hydrodynamic functions (Figure 3.6) as general guides, five sub-classes within the original soil moisture content range (0.22 to 0.63 m/m) were established as fuzzy sets (Figure 3.7). Hence, moisture of any point in the soil profile may be expressed with linguistic variables, namely: Very Wet (VW), Wet (W), Moderate (M), Dry (D), and Very Dry (VD). Second, for any pair of adjacent soil compartments, each with five possible wetness levels, 25 ( $=5 \times 5$ ) different flow classes were defined (Table 3.1). Due to these flow classes, generated data were split into 25 sets and each set was split randomly into training and testing sets (Table 3.2). Third, while the ANN structure was kept constant, 25 specialized ANNs were trained. Performances of these ANNs were evaluated using the different indicators described below.

a. Error ( $D - E$ ) and absolute relative error ( $|D - E| / D$ ) were calculated and plotted versus desired flux, where  $D$  is desired (Darcy-Buckingham) and  $E$  is estimated (ANN) fluxes. These graphs reveal if errors follow a pattern. Root Mean Square sum ( $RMS = [\sum (D - E)^2 / n]^{0.5}$ ) and Mean Absolute sum ( $MA = \sum |D - E| / n$ ) of errors were also calculated and used as lumped performance indicators, where  $n$  is the number of records used for ANN testing.

b. A good match between estimated and desired values is detectable if the scatter diagram shows a 1:1 linear relationship. Forced (through the origin) and free linear regressions, of estimated on desired values, may acceptably substitute the scatter diagram. Hence, regression line 'slope' and 'intercept' were used as performance indicators by comparing them with 'one' and 'zero' respectively. Also, a correlation coefficient was used as another informative indicator jointly with the regression line coefficient(s).

Table 3.1. Flow classes due to upper and lower compartment soil-moisture

Class #	Soil-moisture		Class Code	Class #	Soil-moisture		Class Code
	Upper	Lower			Upper	Lower	
1	VW	VW	A/A	14	M	D	C/D
2	VW	W	A/B	15	M	VD	C/E
3	VW	M	A/C	16	D	VW	D/A
4	VW	D	A/D	17	D	W	D/B
5	VW	VD	A/E	18	D	M	D/C
6	W	VW	B/A	19	D	D	D/D
7	W	W	B/B	20	D	VD	D/E
8	W	M	B/C	21	VD	VW	E/A
9	W	D	B/D	22	VD	W	E/B
10	W	VD	B/E	23	VD	M	E/C
11	M	VW	C/A	24	VD	D	E/D
12	M	W	C/B	25	VD	VD	E/E
13	M	M	C/C				

Table 3.2. Number of records used for training and testing of the ANN modules.

Class #	Records for		Class Code	Class #	Records for		Class Code
	Training	Testing			Training	Testing	
1	562	140	A/A	14	2885	723	C/D
2	179	45	A/B	15	3460	864	C/E
3	296	72	A/C	16	491	125	D/A
4	484	124	A/D	17	1665	417	D/B
5	587	149	A/E	18	2864	715	D/C
6	179	45	B/A	19	4743	1185	D/D
7	256	66	B/B	20	5699	1425	D/E
8	1003	251	B/C	21	531	133	E/A
9	1644	410	B/D	22	1793	448	E/B
10	1958	490	B/E	23	3053	765	E/C
11	299	77	C/A	24	5073	1266	E/D
12	1025	257	C/B	25	6176	1543	E/E
13	1766	442	C/C				

c. Suggested first by Kok et. al<sup>11</sup>, 'SCORE' is a lumped measure of agreement, between 0 (no match) to 100 (complete match). SCORE is a complement to a kind of standardized relative error. The original procedure considers a filtration step to remove high frequency components. In this study, however, in order to make the schedule less conservative, the filtration step was not taken into account.

$$\text{SCORE} = \{1 - [\sum (D - E)^2 / \sum D^2]^{0.5}\} * 100$$

After checking ANN performances and finding them acceptable, a module was coded to simulate the unique ANN structure. For each flux class, the program receives pairs of soil-moisture suctions, then yields flow rates using weights and transformation factors that are extracted from the trained ANN. At this point, the model was ready to be shifted to the next stage, i.e. FIS development.

### **The FIS Module**

Defining soil-moisture classes as fuzzy sets was the very first step in this stage. As aforementioned, the number of fuzzy sets (five), their shape (trapezoidal), and their boundary values (Figure 3.6) were selected based on inspection of the soil hydrodynamic functions (Figure 3.7). These fuzzy sets, in turn, raised (5\*5) 25 fuzzy rules, each leading to one flux class. Without fuzzy sets and FIS, transfer from one flux class to another could produce an abrupt change.

Details of the FIS used in this study are shown in the five steps of Figure (3.8). The first step, fuzzification, interprets the soil moisture contents of soil compartments as fuzzy variables. In fact, comparison of moisture contents with the five soil-moisture fuzzy sets yields five membership values, between 0 to 1. For each compartment, zero indicates irrelevancy of the soil-moisture to the set and a non-zero value expresses the level of soil-moisture affiliation to the set. By way of the second step 'AND' fuzzy operator is used to define DOF for each rule. That is to set the DOF equal to the smallest membership value introduced to the

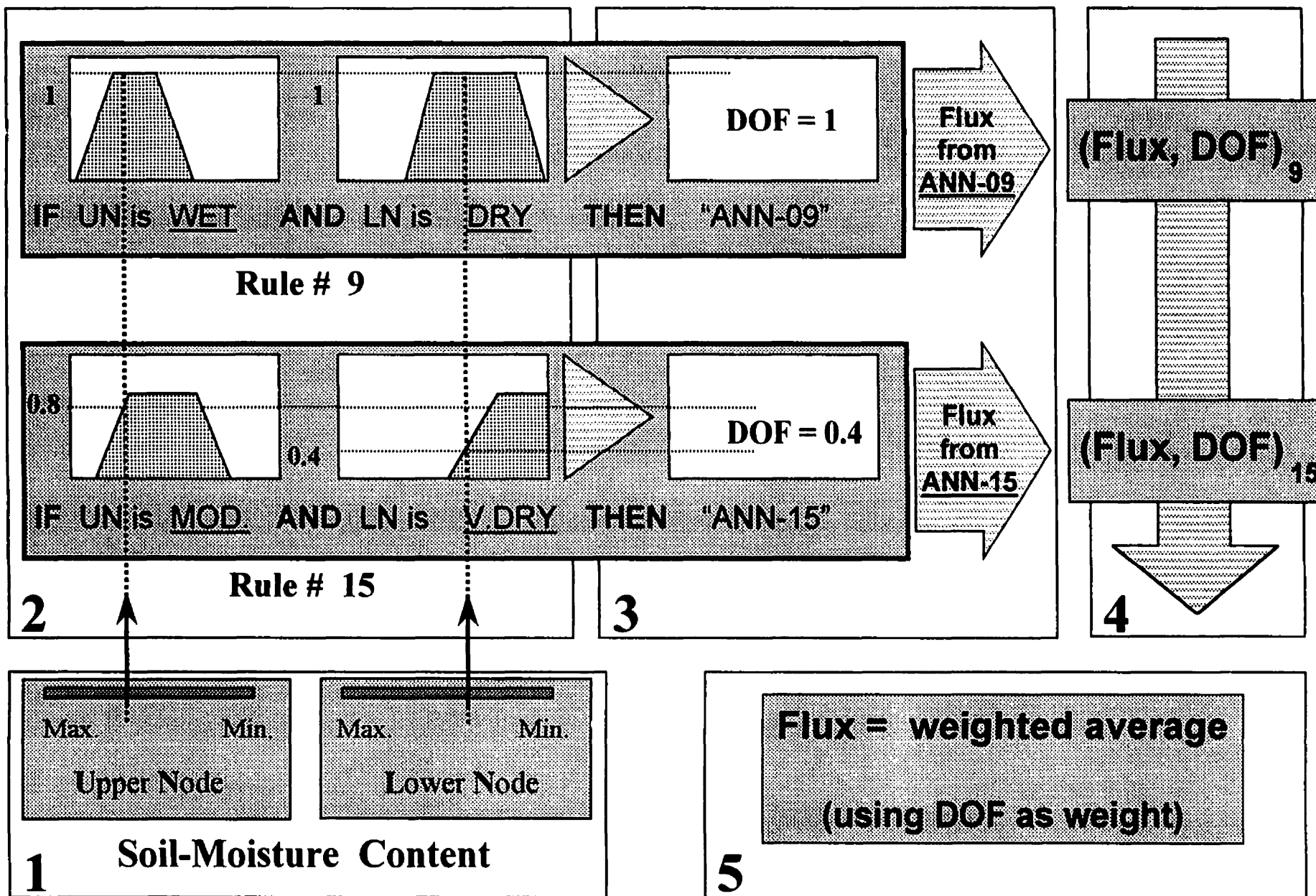


Figure 3.8. An example of the FIS role in flux estimation

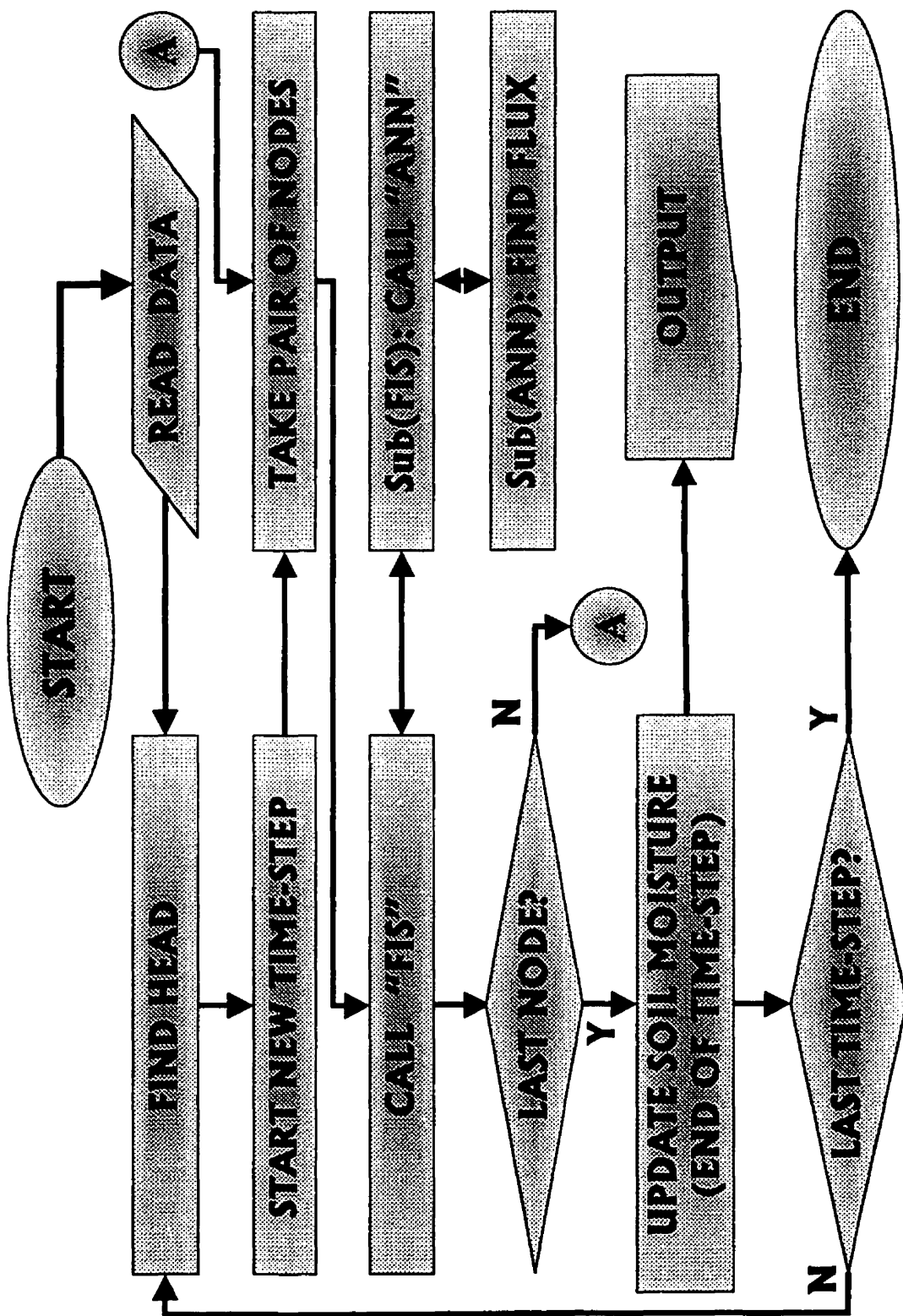


Figure 3. 9. The general flow-chart of the model.



rule antecedent. The third step, implication, executes the rules with non-zero DOF, and yields the rules consequences via excitement of the appropriate ANN and thus getting back their responses, the flux. The fourth step, aggregation, is used to unify or integrate all outputs to make a combined output for the FIS. Finally, defuzzification, employs the Sugeno algorithm to produce a single value flux as the FIS output. As the last step in FIS development stage, a FORTRAN code for the FIS was written to be used as a part of main model. Having the ANN and FIS ready, it was time for development of the main model.

### **The Main Program**

The main program, coded in FORTRAN, employs the ANN and FIS modules while marching through space (flow region) and time (simulation duration) for calculation of the soil-moisture heads and contents. The flowchart presented in Figure (3.9) shows how this task is accomplished. Collectively, the main program with the ANN and the FIS modules constitute the sample model. The new modeling approach is termed “ANN- and FIS-based VSSM redistribution 1D simulation model” and is abbreviated as “ANN-FIS-1D”.

A transient VSSM flow in an assumed soil profile depth of 1.5m, descretized into 31 nodes (30 compartments each 5cm thick), with the following boundary and initial conditions was set as a simple case to test the ANN-FIS-1D model against the SWAP93 model.

$$t = 0 ; S_i = 3 \text{ m } (1 \leq i \leq 31)$$

$$t > 0 ; S_1 = 15 \text{ m and } S_{31} = 3 \text{ m}$$

Where:  $t$  is time,  $i$  is the node number, and  $S$  is the soil suction. The results are presented and discussed below.

Table 3.3. Performance indicators for the ANN modules

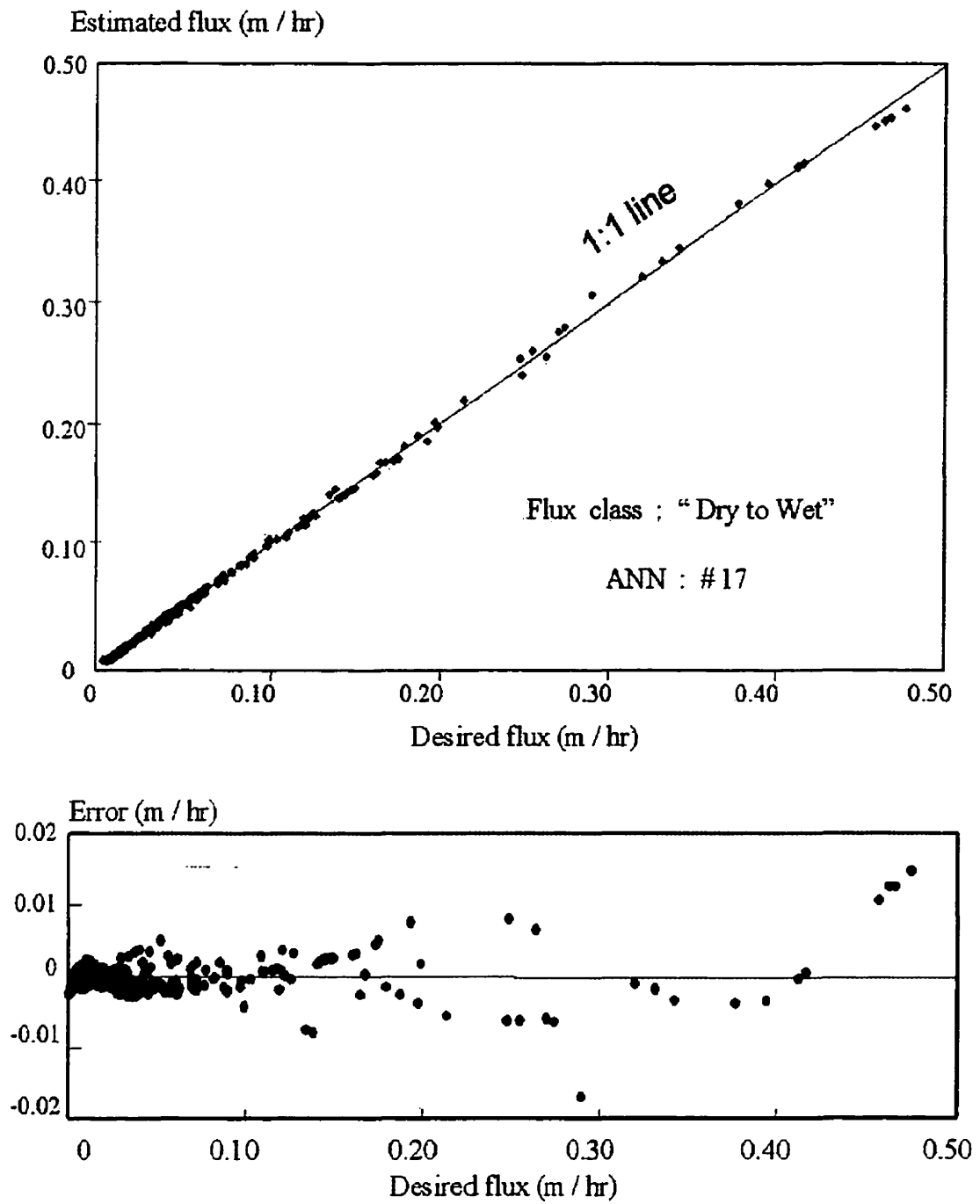
Row #	Flow Class	Regression Parameters		Correl. Coeff.	RMS	SCORE
		Const.	Slope			
Ideal value =>		0	1	1	0	100
1	A/A	0.023031	1.001899	0.9992	0.46668	96.17
2	A/B	0.051445	0.999606	0.9992	0.46867	96.80
3	A/C	-0.010408	1.000007	0.9997	0.29756	98.18
4	A/D	-0.018623	0.999738	0.9999	0.19603	99.18
5	A/E	-0.001975	0.999814	0.9998	0.30769	98.81
6	B/A	-0.047898	0.988403	0.9993	0.47683	96.12
7	B/B	-0.050920	0.977096	0.9964	0.72246	91.52
8	B/C	0.000350	0.996809	0.9994	0.27364	96.83
9	B/D	-0.081167	0.995672	0.9993	0.40947	96.61
10	B/E	-0.021805	0.996727	0.9997	0.32579	97.82
11	C/A	0.041014	0.993804	0.9993	0.17549	97.80
12	C/B	0.032851	0.988288	0.9972	0.29471	93.49
13	C/C	0.001050	0.995010	0.9992	0.01116	95.91
14	C/D	-0.000542	0.996658	0.9996	0.00988	97.67
15	C/E	-0.000971	0.995923	0.9994	0.01449	97.39
16	D/A	0.010080	1.000186	0.9999	0.17340	98.91
17	D/B	0.042174	0.994226	0.9996	0.23651	97.36
18	D/C	0.000955	0.995465	0.9994	0.01044	97.03
19	D/D	0.000116	0.996933	0.9996	0.00453	97.33
20	D/E	-0.000335	0.998126	0.9997	0.00306	98.38
21	E/A	0.040737	0.997949	0.9998	0.26353	98.66
22	E/B	0.011512	0.995778	0.9989	0.42309	96.01
23	E/C	0.002312	0.993424	0.9993	0.01254	97.48
24	E/D	0.000304	0.998886	0.9996	0.00332	98.23
25	E/E	0.000126	1.008498	0.9993	0.00330	96.16

## RESULTS AND DISCUSSION

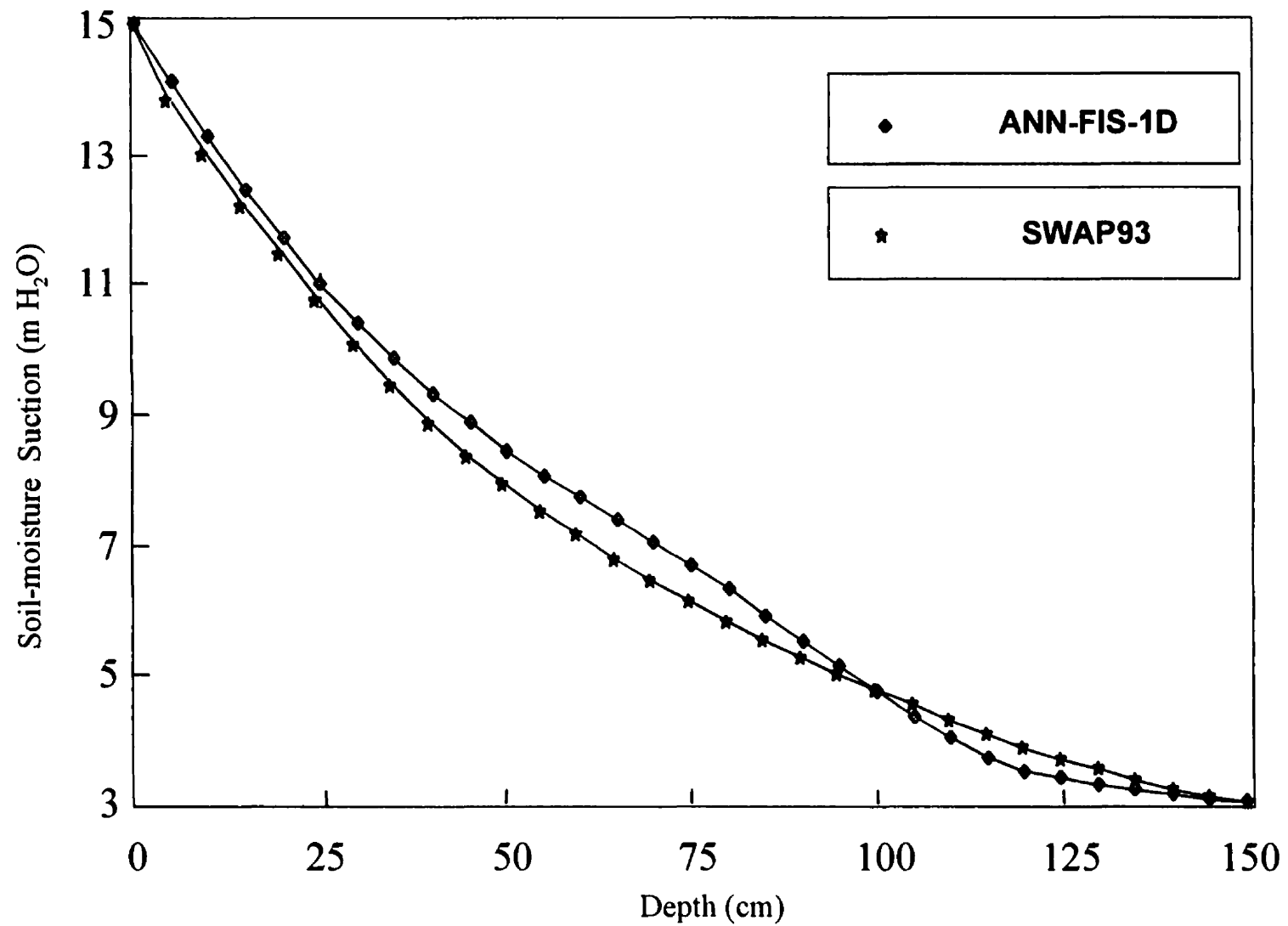
From the literature data, plotted in Figure (3.6), it is obvious that the behavior of the curve slopes contradict each other. In fact, this makes the Richards' equation difficult to solve numerically. These graphs were used as general guidelines for selection of the boundaries and shapes of the fuzzy sets. Choice of fuzzy set ranges can have an impact upon model results. Defining a large number of sets may alleviate the problem, but this leads to laborious program coding and lengthy computation time. One way to select suitable ranges for fuzzy sets, as was employed in this study, is to emphasize physical guidelines, such as soil hydrodynamic functions, and use trial and error.

The performance of the 25 ANN modules were monitored via several performance indicators (such as regression coefficients, correlation coefficient, RMS, and SCORE) reported in Table 3.3. Also, plots of estimated vs. desired fluxes (to visualize the match between the two) and errors vs. desired fluxes (to track any non-random trend in the errors) were used. The plots, presented in Figure (3.10), reaffirmed the results of Table 3, strengthening approval of the ANN modules. Two general trends may be noticed in the error plots. First is an increase in the absolute error as the flux increases. Yet, this coincides with a decreasing trend in the relative error. Second, is an apparent sinusoidal trend in Figure (3.10). This is a result of the non-uniform distribution of the training data.

Next, the ANN-FIS-1D model and SWAP93 models were executed for a 30-day simulation period and outputs were compared. After the 12th day results show that steady state, under constant boundary conditions, had been re-established. A good match was found between the models (Figure 3.11) with a maximum error of less than 8%. The error magnitude should be assessed cognizant that the level of inherent uncertainty in VSSM flow input parameters is usually much higher. The satisfactory result of the sample model demonstrates the acceptable



**Figure 3.10.** Performance of ANN-17; Top: estimated versus desired fluxes; Bottom: Error versus desired flux.



**Figure 3.11.** Overall performance of the model: comparison between the model and SWAP93 results.

performance and the capability of the ANN-FIS-1D approach for simulation of VSSM flow.

An unsaturated hydraulic conductivity function, an input to conventional models such as SWAP93, was not required for the ANN-FIS-1D based model. In fact, reducing the number of inputs is an advantage of the ANN-FIS-1D approach that may generally be called 'input simplification'. Two other possible ways for input simplification are acceptance of soil structural and textural properties instead of soil hydrodynamic parameters, and application of qualitative variables. Another expected advantage of the ANN-FIS-1D approach over conventional numerical methods is less computational time especially for more complex (2D, 3D, non-homogeneous) cases. Potentially, ANN-FIS-1D is very promising but at least in the short term, is not a complete substitute for numerical models. A universal and fully operational version of a ANN-FIS-1D model, including all its expected advantages, may become accessible whenever a comprehensive soil/VSSM database becomes available for training.

## **CONCLUSIONS**

ANN-FIS-1D, a new VSSM flow modeling approach that applies FIS and ANN techniques, was introduced and its basic concepts and components discussed. Based on this approach, a transient VSSM 1D flow model was developed and tested for comparison against SWAP93, and a good match was found between the two models results. The maximum error was less than 8%. The satisfactory performance of the sample model demonstrates the potential capability of the ANN-FIS-1D approach for simulation of VSSM flow.

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## **CONNECTING TEXT: CHAPTERS THREE & FOUR**

Chapter three demonstrated the ANN-FIS-1D simulation model. The ANN was trained to estimate a flux between two adjacent nodes based on their soil moisture heads. To enhance the ANN estimations, 25 specialized ANNs were trained (instead of one) and combined via FIS.

While developing the ANN-FIS-1D approach, a totally different point of view emerged with regards to the use of an ANN for the VSSM redistribution modeling. This alternative approach, ANN-1D, is presented in chapter four. The ANN for this method was trained to estimate soil moisture heads for a whole soil profile based on antecedent moisture and boundary conditions. Inasmuch as the boundary conditions are given to the ANN it was possible to train the ANN for larger time steps (equal to boundary conditions renewal intervals). In fact, the ANN-FIS-1D and ANN-1D are two completely different approaches which are almost in total contrast with each other. These methods are compared and contrasted in chapter 6.

## **CHAPTER FOUR: THE SECOND 1D MODEL**

**ABSTRACT:** This chapter explains two nearly related non-numerical modeling approaches for variably saturated soil moisture (VSSM) movement. Both methods employ artificial neuronet (ANN) technique to find soil profile moisture upon receiving the soil profile antecedent moisture pattern, as well as present and previous boundary conditions. SWAP93 model, which is based on Richards' equation, was employed to generate daily data for ANN training task. The trained ANNs, then, evolved into one-dimensional unsteady VSSM flow models that require less detailed input. The models simulate soil profile moisture redistribution, stepwise and forward through time, and their output compared with that of SWAP93, and good matches were found. Overall, in comparison to the variance usually associated with VSSM parameters, the errors seem quite acceptable.

### **INTRODUCTION**

Variably Saturated Soil Moisture (VSSM) flow models can be used as planning, designing, and managing tools for irrigation/drainage or any other soil-water related process. Often, they are used to simulate alternative scenarios to provide more insight into likely benefits and drawbacks.

Common practices in VSSM flow modeling are based on numerical solution of the Richards' equation. However, numerical solutions are associated with many programming efforts and often have high computation costs. Also, results are inherently combined with high uncertainty due to temporal/spatial diversities, intrinsic to the VSSM input parameters. For instance, unsaturated hydraulic conductivity, an important input parameter, is a function of soil type and also is a function of soil moisture with sharp variations. Unsaturated hydraulic conductivity is rarely measured, but is usually estimated. At best, the function is

estimated from point-measured values of “saturated hydraulic conductivity” and “a soil moisture retention function”; where the latter one is usually measured from disturbed soil samples in the laboratory. These problems contribute to model uncertainty to an extent that results of the models can only be regarded as approximations of reality<sup>1</sup>.

To circumvent these problems the authors presented an ANN-based VSSM model. This approach lowers programming efforts as well as facilitates the preparation of inputs via acceptance of 'soft' data and a decrease in the number of inputs. The model development, as reported in this chapter, was based on two other steps. First, data were generated via Richards' equation. Second, two ANNs were trained to estimate soil profile moisture distribution. Then, two transient one-dimensional (1D) models were developed that utilize the ANN -at any time step- to compute final soil profile moistures. This chapter explains both models and their results. Results of the two models were compared with SWAP93<sup>6</sup> outputs.

### **THE IDEA, PROS AND CONS**

Non-numerical solutions for VSSM flow are favored if they overcome the problems associated with numerical solutions. The idea introduced in this chapter leads to a very lucid code. And inasmuch as its computation cost is very small, the sample models presented here were executed at least three times faster than that of SWAP93. The method has, also, the potential to employ real world data (VSSM flow observations) for ANN training. This offers the idea that estimation of the highly uncertain VSSM flow parameters can be bypassed.

Inasmuch as these models are non-numeric with no iteration, utilizing the trained ANNs within the entailed ranges, their computation is speedy and stable. Although results of any model are approximations, but errors of tested sample models are small and reasonable compared to uncertainties associated with

numerical flow models. Besides these pros, the model has some cons too. An important one is the fact that the trained ANN does not pay attention to preservation of mass; therefore, correction of minor imbalances –at the end of any time step– need separate consideration. Another disadvantage is the long time and tedious efforts needed to train ANNs for such nonlinear cases. In fact, if a comprehensive data set is available the time and efforts needed to train an ANN, as an ‘universal VSSM flow estimator’, might pose a serious barrier. However, such an estimator would be fast, would promote uncertainty handling, and would facilitate the input preparation.

## **MODEL DEVELOPMENT**

The approach suggested in this chapter is demonstrated via sample models through simulation of some unsteady VSSM flow cases. Development of sample models had three distinct stages, namely: data generation, ANN training, and model implementation. Hereafter, for convenience, the two sample models are called M1 and M2. The main difference between M1 and M2 is due to the representation of soil-water distribution by their ANN modules. While M1 employs an ANN (M1-ANN) that provides soil-water heads at 10 equally spaced nodes, the ANN module of M2 (M2-ANN) returns coefficients of a 5<sup>th</sup> degree polynomial that describes the soil-water distribution (in term of head) through the soil profile. More details of both ANNs are given later on. Performance of M1 and M2 has been tested and compared with the results of SWAP93<sup>6</sup> model, an offspring of the well-known SWATRE<sup>2</sup> model. While the results are presented at the end of this paper, the subsequent sections provide details on the three modeling stages.

### **Data Generation**

Data generation was the first step in this study. Original soil data for this study was taken from a table in DRAINMOD reference report<sup>5</sup> that contains soil

moisture 'content', 'head', and 'unsaturated hydraulic conductivity' records. Assuming 10 different profile depths (from 25cm to 250cm), each discretized to 10 equal compartments, along with 12 initial conditions (uniform and non-uniform soil moisture heads from -200 to -7000 cm-H<sub>2</sub>O), 5 lower boundary conditions (4 sets of defined daily heads from -200 to -4000 cm-H<sub>2</sub>O, and free drainage), and 8 upper boundary conditions composed of pre-defined sets of daily potential soil evaporations (from 0.05 to 0.95 cm) and daily rainfalls (from 0.00 to 2.00 cm), all together 4800 ( $=10 \times 12 \times 8 \times 5$ ) separate input files were prepared for SWAP93 model. The simulation period was set to 25 days and SWAP93 was executed for all input files. Simulation outputs were saved at the end of each simulation day.

For M1-ANN pairs of 10 nodal soil-water heads -for any two successive days- extracted from SWAP93 output files, along with boundary conditions form records that were arranged in new files with a suitable format for ANN training task. Inasmuch as pairs of daily heads (initial state and desired output at any time step) are needed for each record, total records produced was 115200 ( $= [25 - 1] \times 4800$ ) lines.

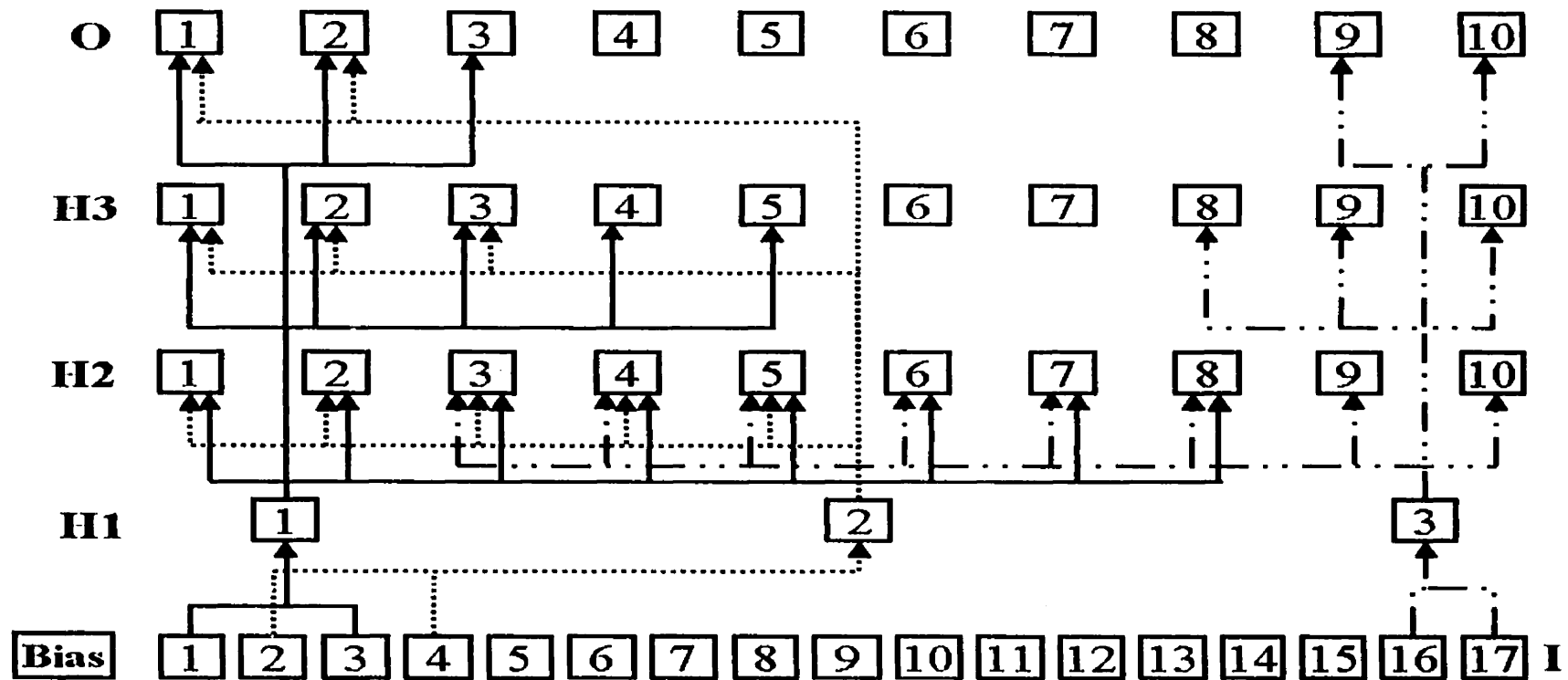
M1-ANN was trained to predict 10 head values at uniformly spaced nodes through the soil profile. For training purpose, desired outputs for the ANN were 10 final nodal heads. Inputs are composed of 10 initial nodal heads, 4 initial and final upper boundary conditions (includes rainfalls and soil potential evaporations), 2 initial and final lower boundary conditions (heads at the bottom of the soil profile), and soil compartment thickness. Then each record is composed of 27 values. All together 115200 record lines were extracted and prepared. Furthermore, the data were randomly assigned to three separate files as follow; 58491 lines or 50.77% of records for training, 27878 lines or 24.20% of records for testing, and 28831 lines or 25.03% of records for verification use (target percentages were 50, 25, and 25).

To make the ANN module capable of prediction of heads anywhere within the soil profile, 10 nodal values can be substituted by coefficients of a polynomial that expresses 'head' as a function of 'depth' ( $h = f[z]$ ). To find the best-fit polynomial degree, veracity of polynomials of degrees three to seven was checked and the best-fit was found a 5<sup>th</sup> degree polynomial (with six coefficients). Then, M2-ANN was trained to predict these six coefficients that represent moisture distribution in the soil profile. Inputs are exactly as those of M1-ANN, mentioned above. However, outputs are just those six coefficients, which leads to record lines of 23-value length each. Using extracted records for M1-ANN, a polynomial was fit to each set of 10 final head values (each record) and coefficients obtained were substituted as desired outputs instead of final heads.

### **ANN Training**

Having the training data ready means the number of input layer nodes (17) and output layer nodes (10 and 6) for neuronets are known. However, to find the best ANN architecture (i.e. number of hidden layers and neurons, and the way they are connected) many experiments on several ANN architectures were performed. ANN modules were trained with 'Neural Works Professional II/Plus', version 5.23, software<sup>4</sup>. 'Normalized cumulative delta learning rule' and 'sigmoid transfer function' were found best via trial and errors, and used in all neurons. While training, neuronet 'weights' and overall 'root mean square' (RMS) error for testing data set was used as training performance indicators/controllers, and eventually RMS error for verification data set was used. Noteworthy is that RMS values, as calculated by the software, are lumped (for all ten outputs together) performance indicators and for the scaled (between 0 and 1) data.

Preferred structure for M1-ANN, only with its particular connections (for the sake of clarity standard connections are not shown), is shown in Figure (4.1). The [layer(node), ...] structure may also be given in a linear format as: [I(17), H1(3),



**Figure 4.1.** The ANN and the selective connections. There is no other connection between I and H1 other than what are shown here. There are full connections between I(nodes 5 to 15) and H2, H2 and H3, and H3 and O.

H2(10), H3(10), O(10)]\*. Preferred structure for M2-ANN has only standard connections and in linear format is given here: [I(17), H1(12), H2(10), H3(8), O(6)]. While training, these two ANNs were approved and preferred over other ones not only due to small lumped RMS values based on scaled data, but also due to satisfactory values of other error indexes which are based on unscaled data. These error indexes, performed after training, are described below.

Node-wise errors are checked to make sure that errors are almost the same throughout the soil profile. Linear regressions, forced-through-origin ( $Y=b \cdot X$ ) and simple ( $Y=a+b \cdot X$ ), were performed to check 1:1 relationship between ANN outputs ( $Y$ ) and desired outputs ( $X$ ). A perfect 1:1 match would have a slope ( $b$ ) equal to one, an intercept ( $a$ ) equal to zero. Correlation coefficients, a measure of paired data scattering with a value of one for perfect case, were also calculated. Mean absolute error (MAE) and RMS values are other node-wise error measures that are calculated due to following definitions.

$$MAE = [\sum |D - E|] / n$$

$$RMS = \{ [\sum (D - E)^2] / n \}^{0.5}$$

Where  $D$  and  $E$  are desired and estimated soil moisture heads respectively, and  $n$  is the number of records. In addition, 'SCORE'<sup>3</sup>, a lumped measure of agreement, was also calculated. In the original procedure for SCORE to remove high frequency components a filtration step is considered. In this study, however, in order to make the schedule less conservative the filtration step was not taken into account. The formula used for SCORE is defined below, where it yields 100 for a perfect mach.

$$SCORE = \{1 - [\sum (D - E)^2 / \sum D^2]^{0.5}\} * 100$$

---

\* [Layer(node #), ....]; I: input, H1: hidden1, O: output.



Values found for these error indicators are reported under results and discussions. After the approval process, preferred ANNs were coded as soil-water head estimation modules and made ready for the next (model implementation) stage.

### **Model Implementation**

To march through time and simulate soil-water distributions - using ANN modules at any step - two computer models (M1 and M2) were coded. At each time-step, known initial and boundary conditions are used by the main programs to excite ANN modules and receive their responses; which are 10 new soil-moisture heads for M1-ANN and six coefficients for M2-ANN. In the latter case a fifth degree polynomial is used to find new soil-moisture heads at 10 uniformly spaced internal nodes.

Before leaving the current time step, another module checks the soil-moisture balance for the whole soil profile ( $\Delta\text{storage} = \Sigma\text{input} - \Sigma\text{output}$ ) and corrects minor imbalances, if there are any. Imbalances at each time step were not noteworthy due to the ANNs small errors. Over time, however, imbalances may amplify themselves through repetitive calculations. The corrective measure assumes that the final soil-moisture distribution pattern is correct. Therefore, to abolish the imbalance quantity, it is distributed to all nodes, not uniformly, but imitating the soil-moisture pattern. As an example a large corrective share is assigned to a wet node and a small one to a dry node. Other corrective measures were also tried, but the best result was found using the aforementioned method. The sample models outputs were tested against that of SWAP93 model and good matches were found. The results are presented and discussed next.

### **RESULTS AND DISCUSSION**

The preferred M1-ANN and M2-ANN, each with three hidden layers, had achieved to scaled data RMS values equal to 0.0167 and 0.0134 respectively.

**Table 4.4.** M1-ANN performance indicators for training data set.

<b>N</b>	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-405.1	0.784	0.841	0.923	615.3	261.6
2	-202.0	0.877	0.943	0.952	236.2	159.2
3	-137.8	0.913	0.962	0.969	175.8	119.7
4	-88.4	0.947	0.979	0.984	118.7	80.4
5	-68.5	0.961	0.983	0.988	90.6	57.8
6	-61.8	0.964	0.988	0.990	86.4	55.2
7	-81.7	0.947	0.982	0.983	108.4	72.1
8	-116.1	0.917	0.967	0.968	146.2	100.1
9	-60.5	0.958	0.984	0.984	103.6	78.1
10	-90.4	0.934	0.974	0.978	122.3	95.0

a & b: intercept & slope ( of linear regression ), b': slope ( of regression through origin )  
R: correlation coefficient, RMS: root mean square of errors, MAE: mean absolute of errors

**Table 4.5.** M2-ANN performance indicators for training data set.

<b>N</b>	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-195.5	0.811	0.864	0.945	151.4	87.7
2	-162.1	0.883	0.932	0.958	138.6	85.1
3	-128.6	0.907	0.940	0.966	126.1	77.8
4	-117.0	0.938	0.975	0.978	114.5	69.4
5	-121.1	0.955	0.983	0.989	107.7	73.3
6	-75.0	0.972	0.991	0.994	68.8	54.9
7	-118.3	0.953	0.977	0.980	110.7	67.6
8	-108.9	0.934	0.970	0.971	123.2	75.8
9	-146.7	0.921	0.967	0.965	135.7	83.4
10	-157.2	0.913	0.961	0.953	143.0	86.3

**Table 4.6.** M1-ANN performance indicators for testing data set.

<b>N</b>	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-341.3	0.825	0.877	0.918	588.0	259.2
2	-193.4	0.884	0.946	0.953	233.5	157.5
3	-130.6	0.919	0.965	0.969	174.5	118.8
4	-82.2	0.951	0.982	0.984	118.9	80.2
5	-59.6	0.967	0.990	0.990	91.3	58.0
6	-55.2	0.968	0.990	0.990	85.9	54.9
7	-74.8	0.951	0.982	0.984	107.5	71.8
8	-109.8	0.920	0.967	0.968	146.2	100.2
9	-52.7	0.964	0.987	0.984	102.5	78.0
10	-82.9	0.940	0.976	0.978	121.5	94.6

**Table 4.7.** M2-ANN performance indicators for testing data set.

<b>N</b>	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-208.2	0.807	0.858	0.936	163.1	89.5
2	-180.5	0.851	0.907	0.945	144.3	86.6
3	-135.4	0.893	0.935	0.958	131.6	79.5
4	-106.7	0.940	0.977	0.981	109.5	62.1
5	-77.1	0.962	0.993	0.993	90.4	50.6
6	11.5	1.026	0.997	0.998	59.3	37.3
7	-112.8	0.958	0.982	0.989	102.1	59.6
8	-125.8	0.940	0.976	0.975	118.7	66.7
9	-138.3	0.932	0.971	0.969	125.8	78.2
10	-143.6	0.927	0.968	0.952	132.4	82.9

**Table 4.8.** M1-ANN performance indicators for verification data set.

<b>N</b>	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-386.7	0.798	0.852	0.924	613.3	258.1
2	-195.4	0.882	0.944	0.955	232.0	156.5
3	-135.3	0.916	0.963	0.970	173.5	118.2
4	-87.8	0.948	0.980	0.985	117.7	79.9
5	-65.1	0.964	0.989	0.990	90.3	57.9
6	-60.8	0.965	0.989	0.990	86.1	55.2
7	-79.5	0.948	0.981	0.984	108.4	72.0
8	-111.9	0.918	0.966	0.969	146.3	99.9
9	-56.7	0.961	0.985	0.985	103.4	77.8
10	-85.3	0.938	0.974	0.979	122.5	94.8

**Table 4.9.** M2-ANN performance indicators for verification data set.

<b>N</b>	<b>A</b>	<b>B1</b>	<b>B2</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>
1	-188.7	0.857	0.873	0.943	148.4	79.1
2	-165.2	0.879	0.928	0.955	137.3	81.7
3	-136.8	0.893	0.934	0.961	131.5	80.3
4	-124.4	0.931	0.972	0.977	122.6	62.8
5	-115.3	0.961	0.994	0.991	96.5	70.4
6	-68.7	0.976	0.990	0.995	67.6	48.3
7	-120.2	0.960	0.971	0.975	128.3	72.2
8	-121.3	0.929	0.962	0.968	137.1	74.6
9	-134.1	0.933	0.965	0.966	128.7	73.6
10	-148.8	0.907	0.948	0.951	156.3	79.3

ANNs predictions were also verified in detail with unscaled data via RMS, MAE, SCORE, regression line slope and intercept, and correlation coefficient. These are reported in Tables 4.1 through 4.6 for training, testing, and verification data sets, where each row reports the error for a certain node (1 to 10) in the flow region.

Tables (4.1) to (4.6) also represent correlation coefficients and slopes and intercepts for linear regression lines (forced-through-origin [ $E = b' * D$ ] and simple [ $E = a + b * D$ ]). It is obvious from the tables that regression slopes (forced and simple) and intercepts for all nodes other than first and second nodes (near the top boundary) are very near to one and zero, respectively and proportionally. The correlation coefficients are well close to one too.

Another error indicator used was SCORE as a lumped measure, with a value of 100 for a perfect match. SCOREs related to training, testing, and verification data sets were calculated equal to 89.4, 89.1, and 89.5 respectively for M1-ANN, and 93.8, 93.2, and 92.6 respectively for M2-ANN, which denote good matches for both ANNs.

Due to the nature of ANN training process achievement to uniform error pattern for all ANN outputs may be impossible or very costly. For both M1-ANN and M2-ANN error patterns are obvious from Tables (4.1) to (4.6). Commonly in all tables error is minimum for the mid-profile nodes (#5 and #6); moreover, error is maximum for the upmost nodes (#1 and #2). These may be postulated due to large variation of soil-water heads at the upper flow region (near soil surface, under imposed top boundary conditions), comparing to much milder variations in the mid-profile. In fact at the middle of flow region, nodes 5 and 6, disturbance from boundaries is minimum. In the lower half of the flow region, error patterns for M1-ANN and M2-ANN are different. For M2-ANN, errors get larger toward the lower boundary, which is due to larger variations near the boundary. For M1-ANN, error behavior may be deemed strange around node number eight. Through the course of ANN training, some other tried ANN structures did not

**Table 4.7.** Typical correction calculations.

N	Initial Condition		Final Condition		Correction		
	h (cm)	$\theta$ (cm/cm)	h (cm)	$\theta$ (cm/cm)	$\theta / \Sigma \theta$ %	$\theta$ (cm/cm)	h (cm)
1	-557.635	0.4673	-688.171	0.4651	9.991	0.4646	-712.792
2	-527.387	0.4678	-644.037	0.4658	10.007	0.4654	-668.698
3	-512.696	0.4681	-628.090	0.4661	10.013	0.4657	-652.766
4	-512.910	0.4681	-622.768	0.4662	10.015	0.4658	-647.448
5	-527.184	0.4678	-631.166	0.4660	10.011	0.4656	-655.839
6	-554.756	0.4674	-647.366	0.4658	10.006	0.4653	-672.024
7	-595.205	0.4667	-662.489	0.4655	10.000	0.4651	-687.133
8	-648.525	0.4657	-674.580	0.4653	9.996	0.4649	-699.213
9	-685.140	0.4651	-699.120	0.4649	9.986	0.4645	-723.731
10	-719.265	0.4645	-726.294	0.4644	9.977	0.4640	-749.881

show such an error pattern; however, due to their overall inferior performances they were not approved and therefore omitted. This shows the problem is of 'ANN structure related' kind that might be resolved by doing much more trials to finding a flawless ANN structure. After all, the results of M1 model tests, reported later in this paper, implies that total performance of the model is acceptable. In general, the performance of M2-ANN is better than M1-ANN. Therefore, at this point both ANNs were retained to be used as the soil-moisture estimator modules within the sample programs.

To improve the model accuracy, the corrective module was aimed to eliminate the imbalances in the soil profile moisture (estimated via the ANN). A typical correction calculation is presented in Table (4.7). Any estimation starts from known 'initial and boundary conditions' and the ANN output is the 'final condition'. Both initial and final conditions are in terms of soil-moisture heads ( $h$ ). Then, the first step was to find the soil-moisture contents ( $\theta$ ) for both conditions and all nodes. As the second step the total soil-moisture content/storage (equal to: 70.0272cm, and 69.8260cm; where  $\Delta Z=15\text{cm}$ ) and the bottom fluxes (equal to:  $-0.002915\text{cm/h}$ , and  $-0.002461\text{cm/h}$ ) were calculated for both conditions, initial and final. A daily average bottom flux, and thence daily bottom flow (equal to:  $-0.064509\text{cm}$ ) is calculated. The third step employs the soil profile balance equation to find the Total Moisture Correction (TMC) as follow:

$$\textbf{TMC} = (\text{Moisture inputs} - \text{Moisture outputs}) - (\text{Change in moisture storage})$$

$$\textbf{TMC} = (\text{bottom flux} + \text{rain} - \text{soil evaporation}) - (\text{Final storage} - \text{Initial storage})$$

$$\textbf{TMC} = (-0.0645 + 0.0 - 0.2) - (69.8260 - 70.0272)$$

$$\textbf{TMC} = -0.0633 \text{ cm}$$

Negative and positive signs in TMC denote a need to decrease or increase the final soil-moisture, respectively. The final step was to use the soil-moisture distribution pattern as a guide to dispense the lumped correction to nodes.

Therefore, to find the corrected nodal moisture contents, each node receives a share equal to the percentage of its moisture to that of whole profile ( $= 100 * [\theta / \Sigma\theta]$ ).

At this point, the overall performance of both models, M1 and M2, were tested against SWAP93 model through simulation of two illustrative cases, each for a 25 day period, and comparison of the models results. Soil profile depths equal to 150 cm and 250 cm were assumed for first and second cases, respectively. Boundary conditions (upper and lower) for first and second simulations are given in Tables (4.8) and (4.9), while initial soil-moisture head values for nodes number 1 to 10 (from top to bottom of soil profile) were set to [-2000.0, -1777.8, -1555.6, -1333.3, -111.1, -944.4, -833.3, -722.2, -611.1, -500.0], and [-2000.0, -2666.7, -3333.3, -4000.0, -4666.7, -4500.0, -3500.0, -2500.0, -1500.0, -500.0] centimeters respectively.

Figures (4.2) and (4.3), each composed of 25 daily graphs, visualize continuous moisture alterations through the soil profile for both simulated cases. Each graph compares results of simulations performed by M1, M2, and SWAP93 models. Based on SWAP93 -assumed as observed/desired- outputs RMS and SCORE were calculated for M1 and found equal to 115.23 and 86.11 for the first, and 227.13 and 89.98 for the second case simulated, respectively. For M2, RMS and SCORE were found equal to 54.69 and 93.41 for the first, and 172.78 and 92.38 for the second case simulated, respectively. Overall, these indicators and graphs render evidences on the fact that outputs of M1 and M2 models match well with SWAP93 outputs. However, some features of the output graphs need to be discussed in more detail.

If the daily soil-moisture graphs for M1, especially for the first simulation (Figure 4.2), are inspected in more detail, a minor random serrated behavior can be detected. Inasmuch as ANN is not a mechanistical, but a data-driven modeling



**Table 4.8.** Boundary conditions for the first case solved .

<b>Day</b>	<b>Rain (cm)</b>	<b>Soil Evaporation (cm)</b>	<b>Lower Boundary Head (cm)</b>
1	0.0	0.20	-200
2	0.0	0.25	-250
3	0.5	0.05	-300
4	0.7	0.12	-350
5	1.0	0.10	-400
6	0.4	0.10	-450
7	0.3	0.10	-500
8	1.0	0.10	-550
9	0.0	0.30	-600
10	0.0	0.25	-650
11	0.0	0.35	-700
12	0.0	0.25	-750
13	0.0	0.30	-800
14	0.0	0.35	-850
15	0.0	0.45	-900
16	0.0	0.35	-950
17	0.0	0.25	-1000
18	0.0	0.35	-1050
19	0.0	0.30	-1100
20	0.0	0.30	-1150
21	0.0	0.35	-1200
22	0.0	0.30	-1250
23	0.0	0.40	-1300
24	0.0	0.30	-1350
25	0.0	0.40	-1400

**Table 4.9.** Boundary conditions for the second case solved.

<b>Day</b>	<b>Rain (cm)</b>	<b>Soil Evaporation (cm)</b>	<b>Lower Boundary Head (cm)</b>
1	0.0	0.90	-1400
2	0.0	0.85	-1350
3	0.0	0.75	-1300
4	0.0	0.82	-1250
5	0.0	0.85	-1200
6	1.5	0.10	-1150
7	0.0	0.80	-1100
8	0.0	0.90	-1050
9	0.0	0.90	-1000
10	0.0	0.95	-950
11	0.0	0.95	-900
12	1.5	0.05	-850
13	0.0	0.60	-800
14	0.0	0.85	-750
15	0.0	0.95	-700
16	0.0	0.85	-650
17	0.0	0.75	-600
18	0.0	0.65	-550
19	1.0	0.15	-500
20	0.0	0.80	-450
21	0.0	0.85	-400
22	0.0	0.60	-350
23	0.0	0.70	-300
24	0.0	0.80	-250
25	0.0	0.90	-200

technique these errors should not be surprising. In fact, errors of this kind should not be exaggerated while the overall trend of the model output matches that of desired output and error indicators are satisfactory. On the other hand, M2 curves are smooth and do not show such a behavior. At least to a large degree this is due to utilization of a polynomial curve by M2. Therefore, advantages of M2 over M1 may be stated in three folds. These are superior error indicators, more smooth curves, and capability to produce outputs at any points throughout the soil profile.

Finally, the execution times for models were recorded. This was accomplished on a PC platform with AMD-K6-II processor at 380 MHz for M1. PC platform used for M2 had a P-III processor at 600 MHz. The average execution times found for M1 were equal to 532 ms for SWAP93 and almost 184 ms for the ANN-based model. Almost the same proportion found for M2 and SWAP93 execution times – on P-III platform– with 458 ms and 156 ms, respectively. These results may be affirmed by knowing that the ANN-based models have much less computation steps than that of SWAP93 model.

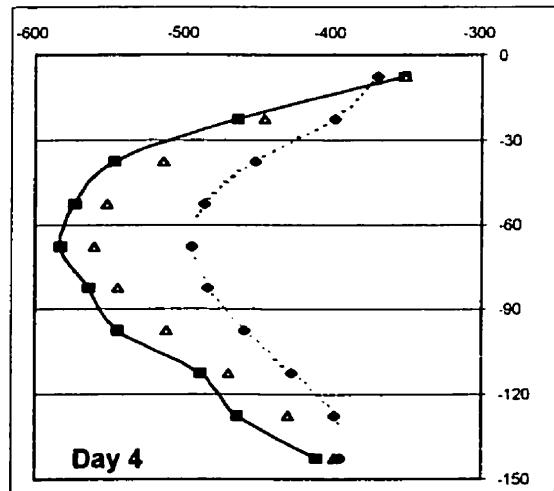
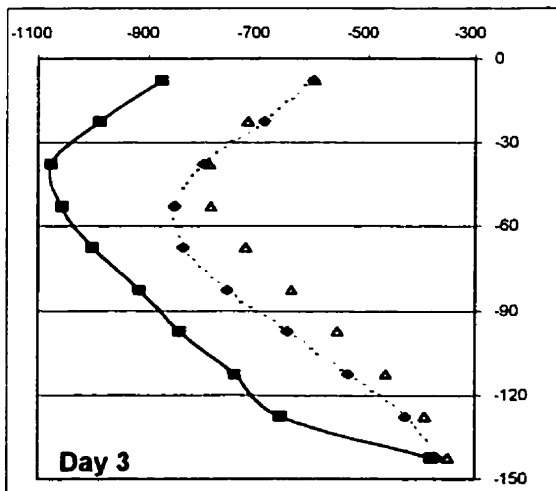
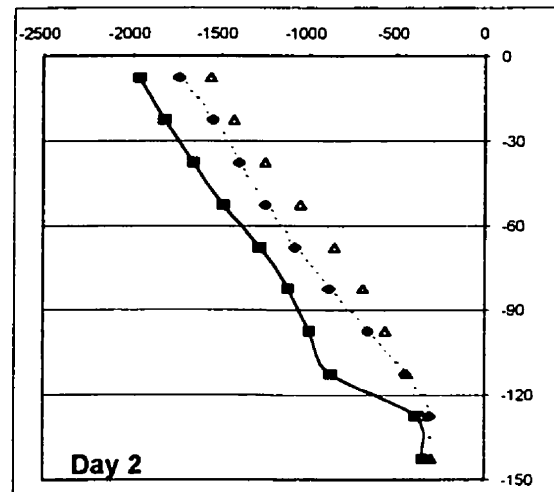
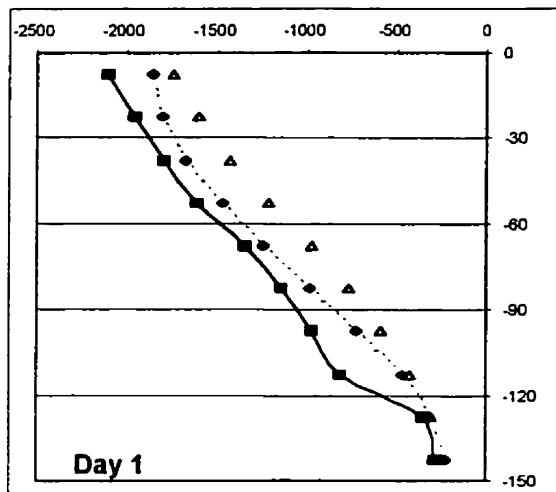
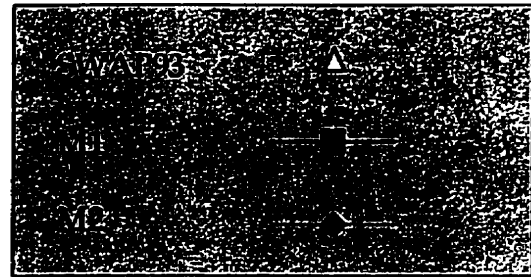
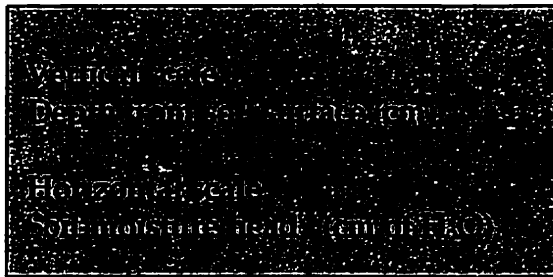


Figure 4.2. Daily results (day 1 to day 25) for the first simulated case.

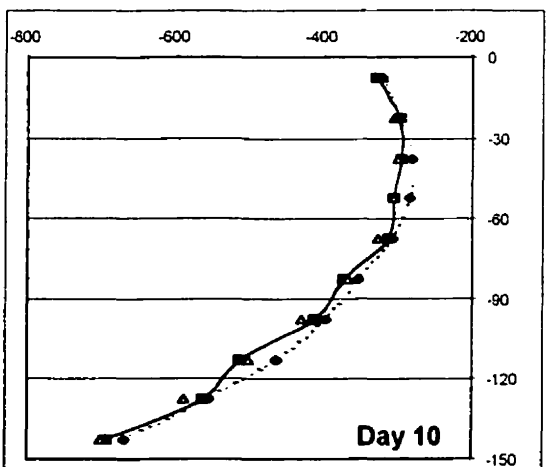
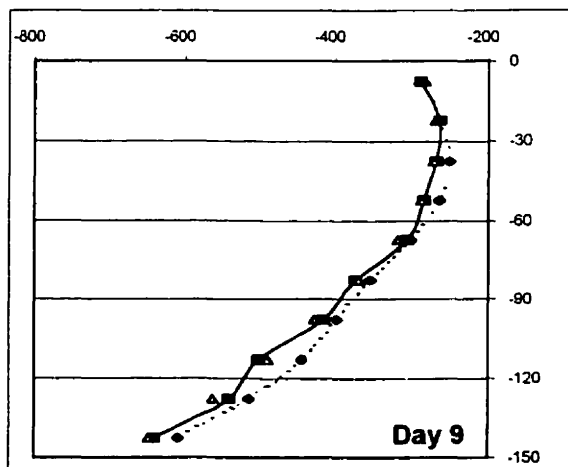
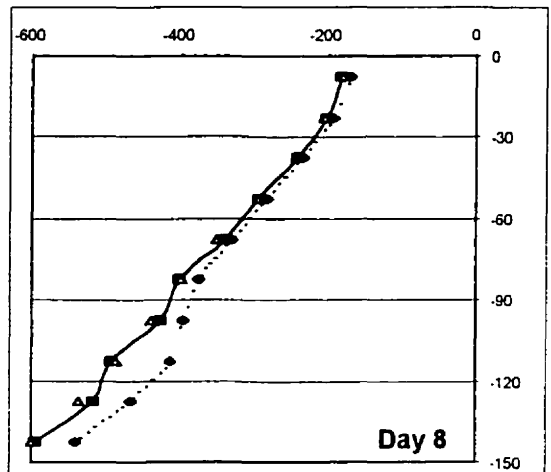
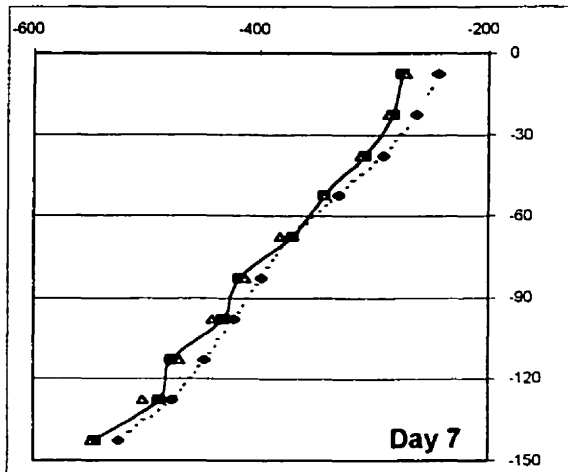
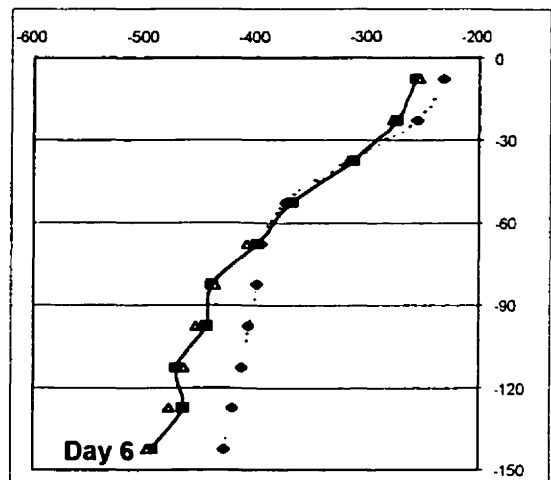
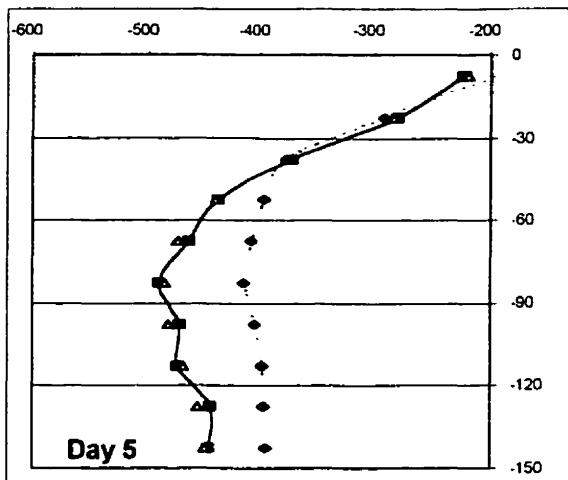


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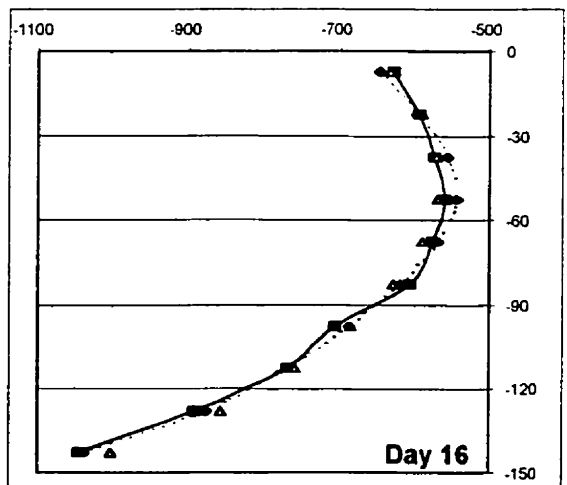
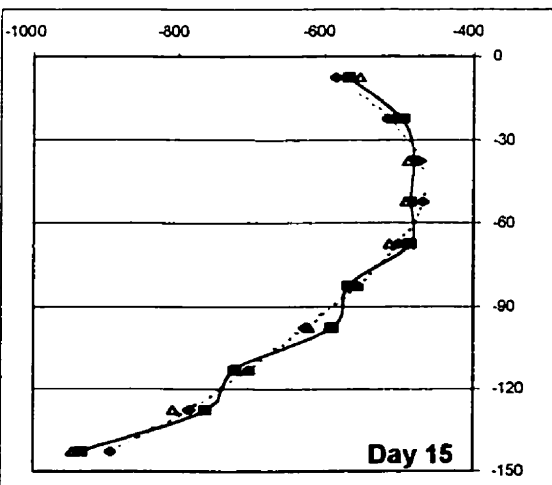
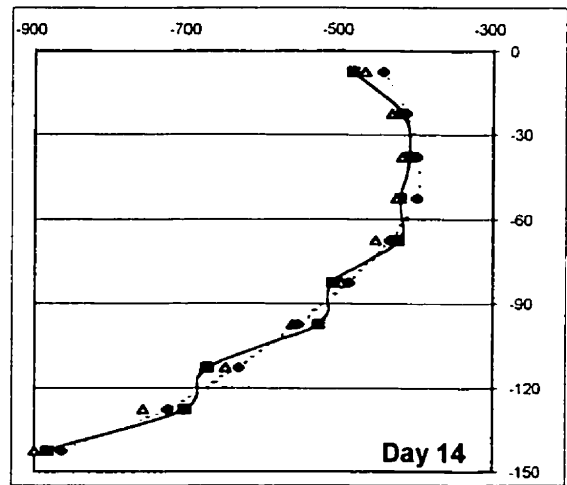
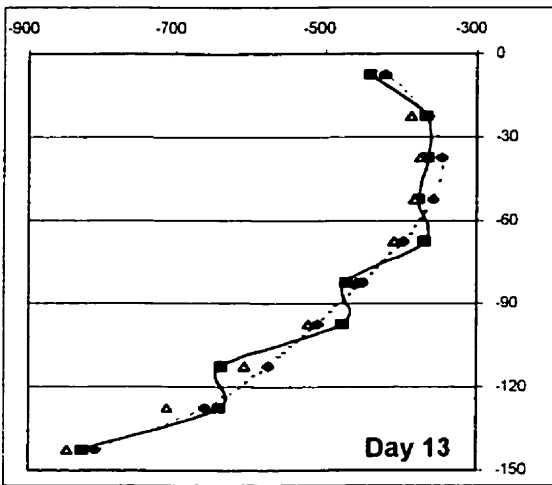
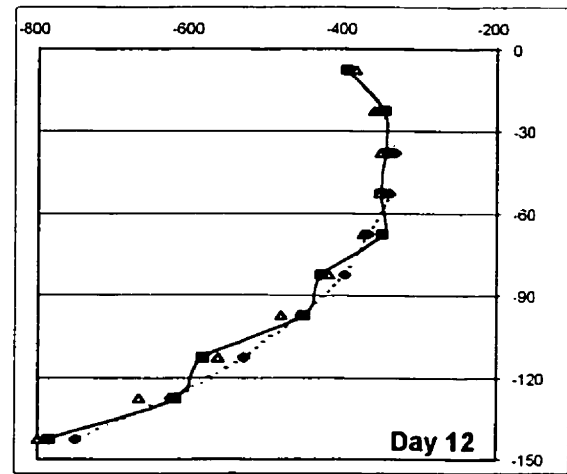
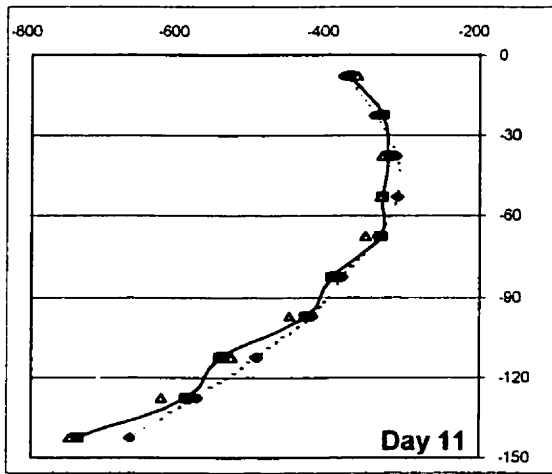


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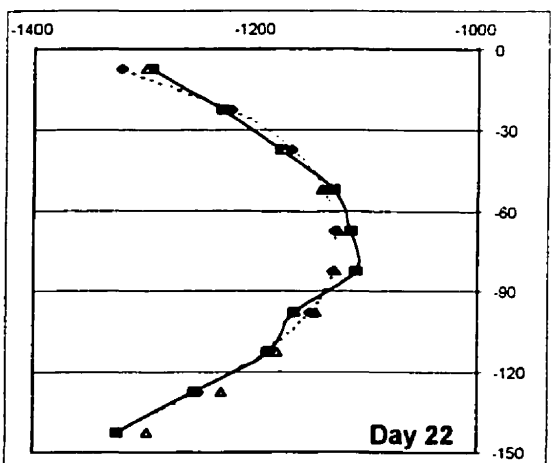
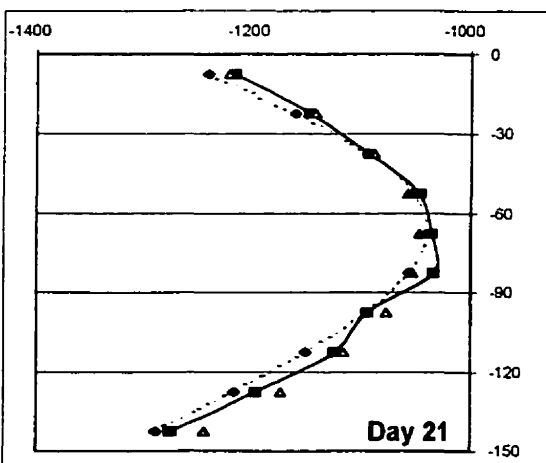
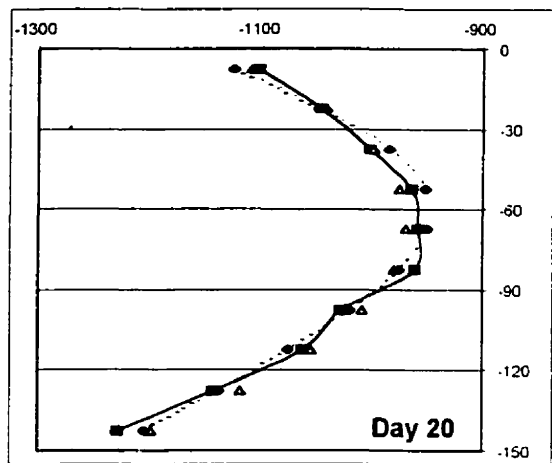
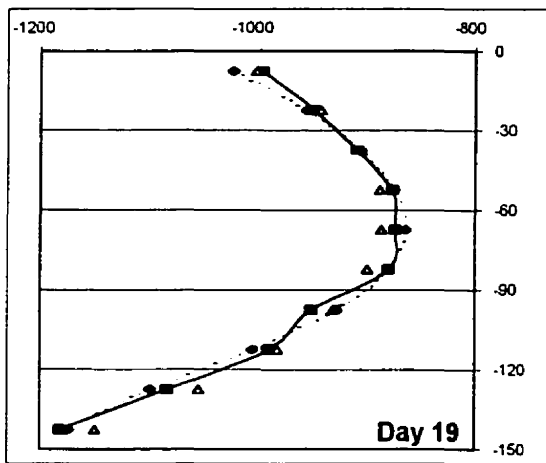
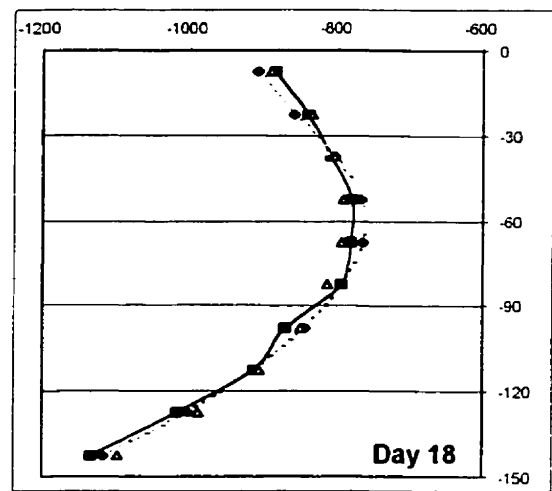
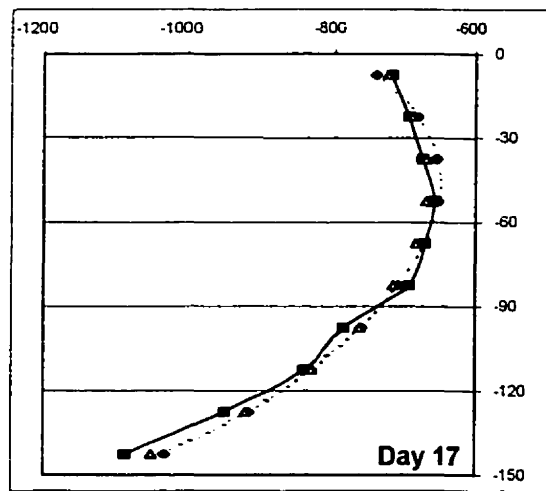


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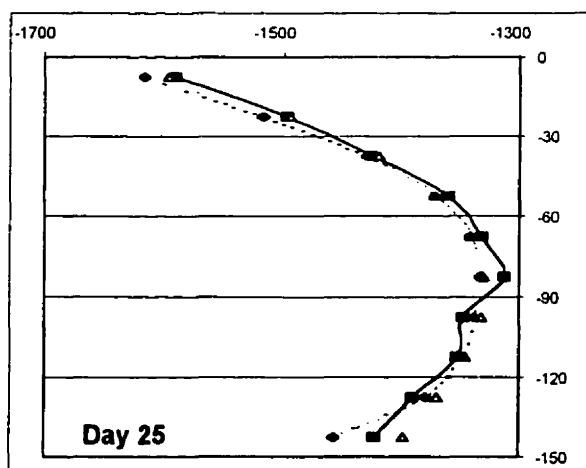
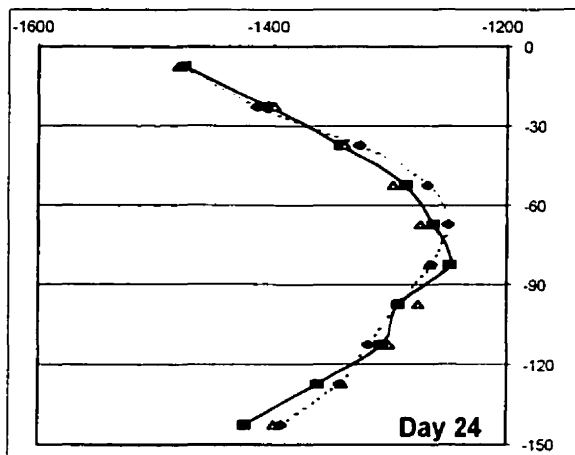
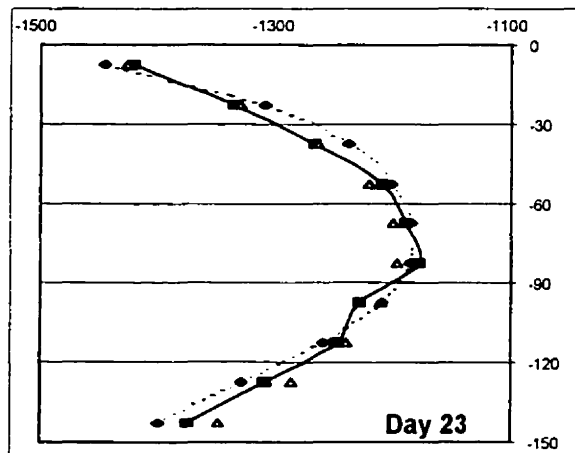


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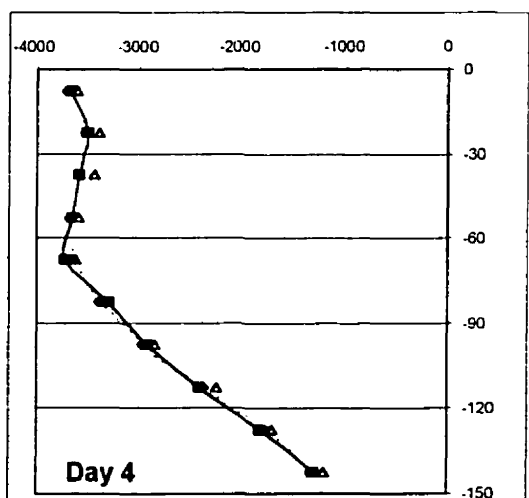
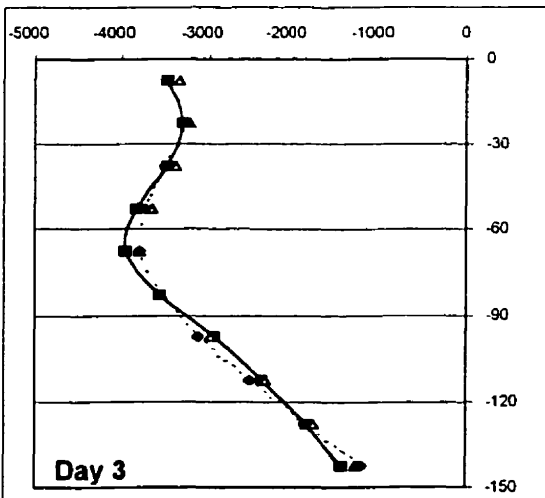
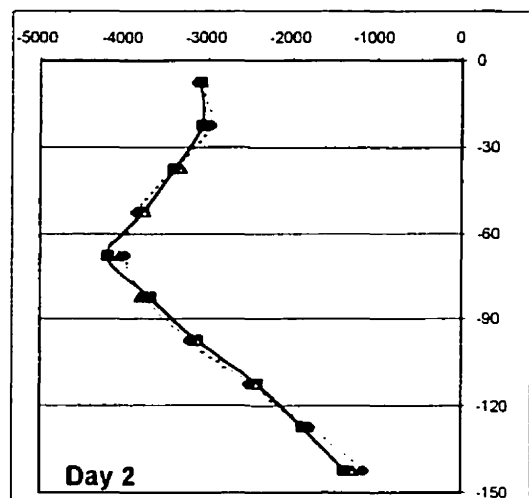
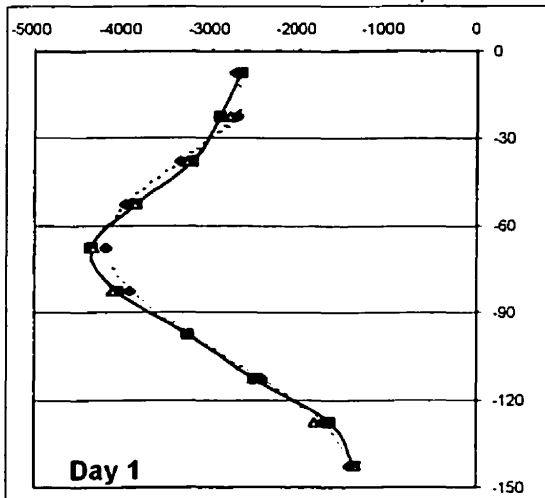
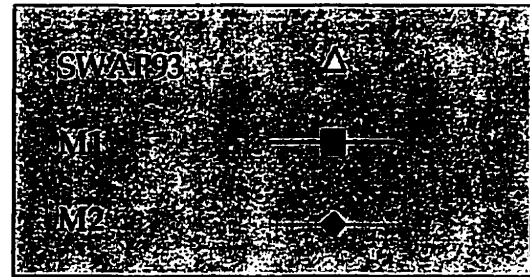
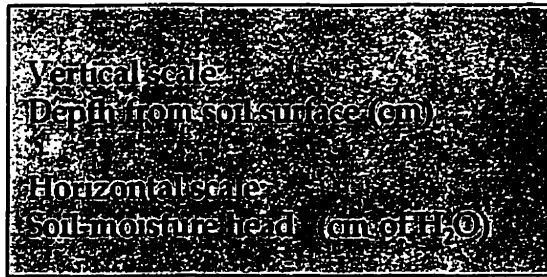
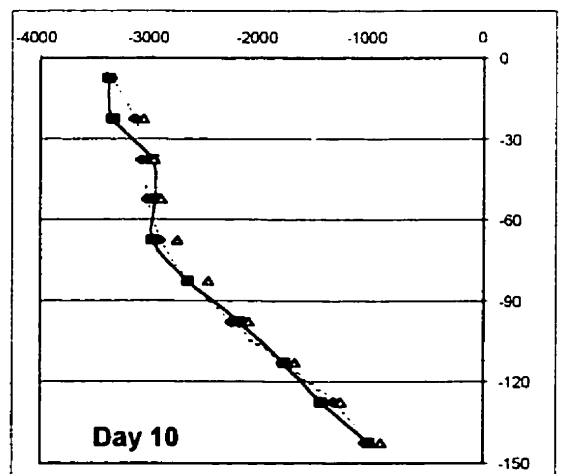
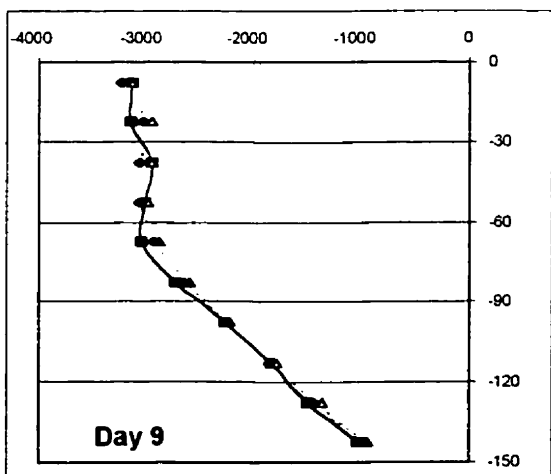
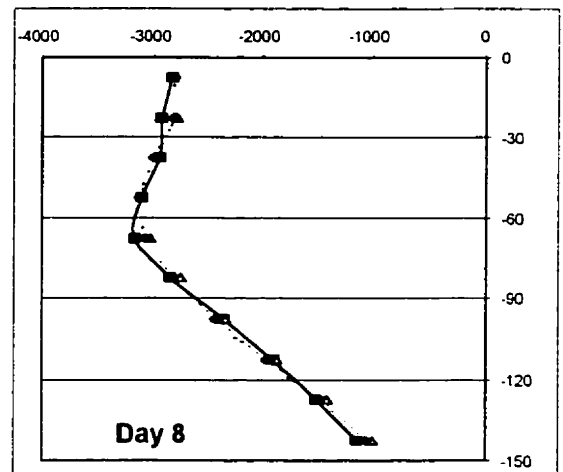
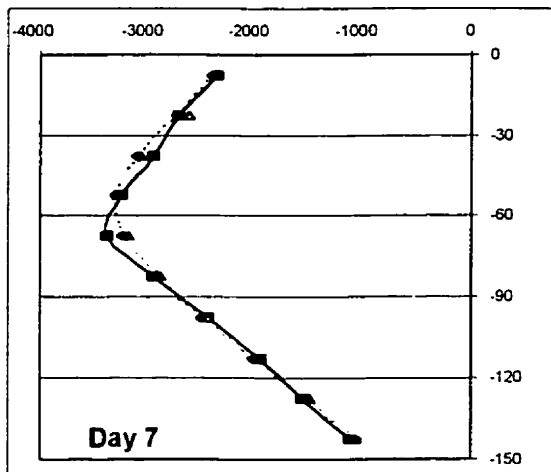
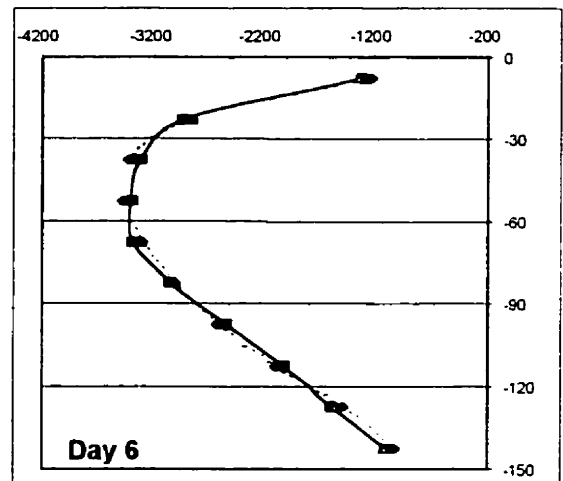
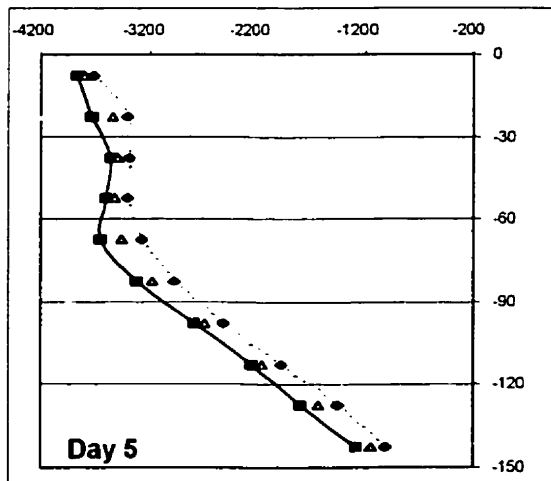


Figure 4.3. Daily results (day 1 to day 25) for the second simulated case.



**Figure 4.3. Continued**

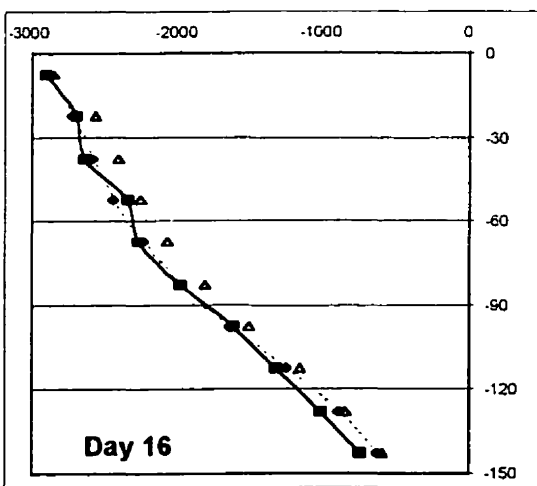
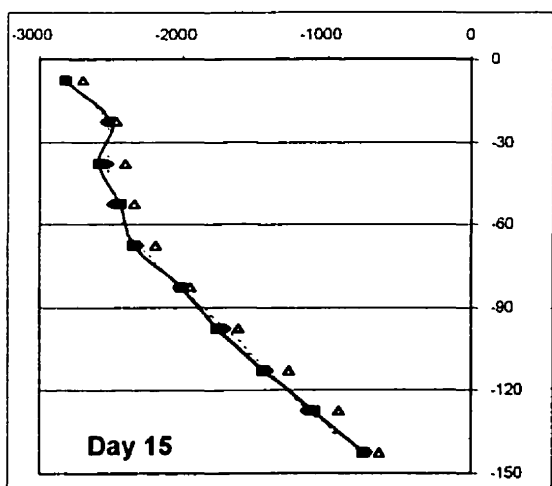
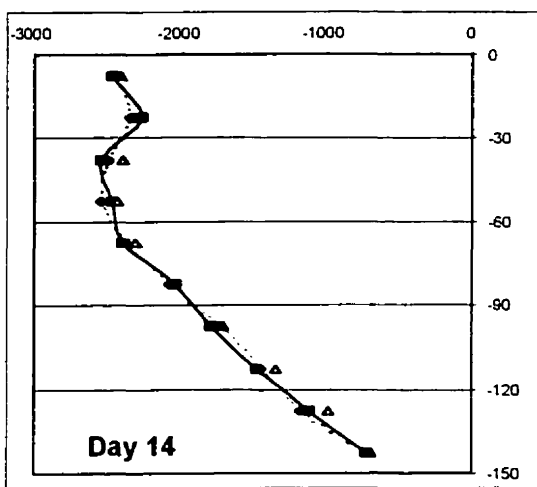
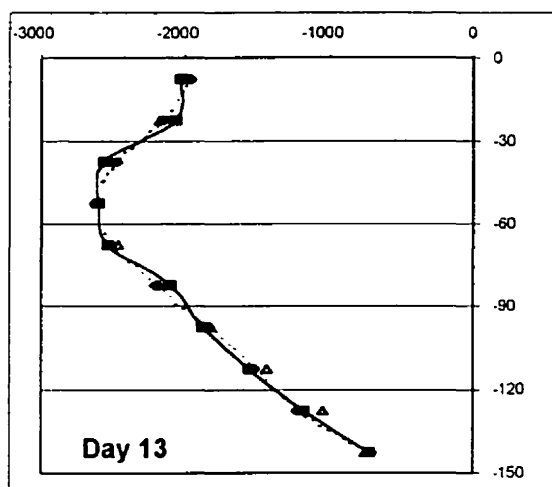
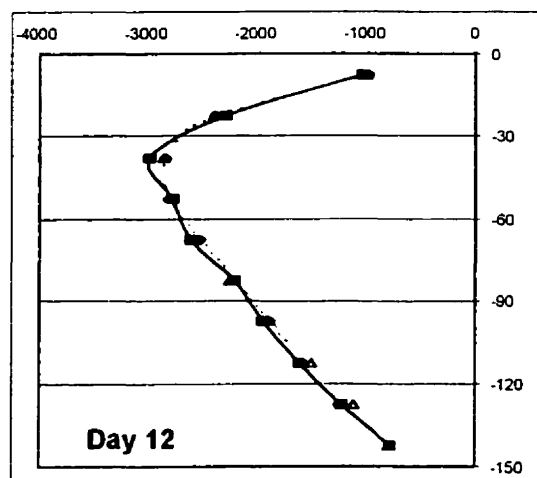
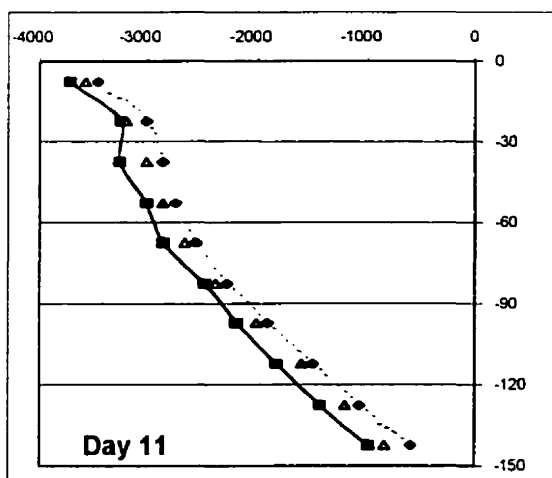


Figure 4.3. Continued

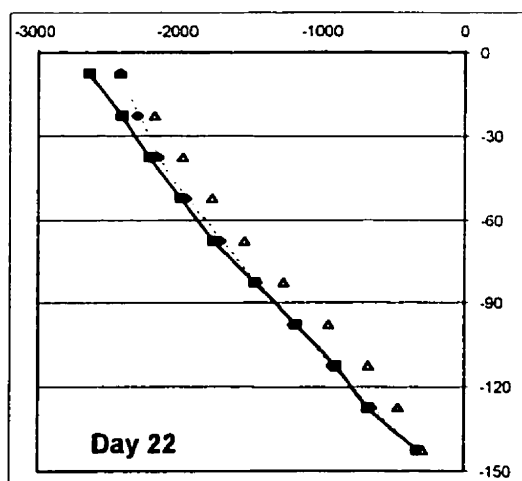
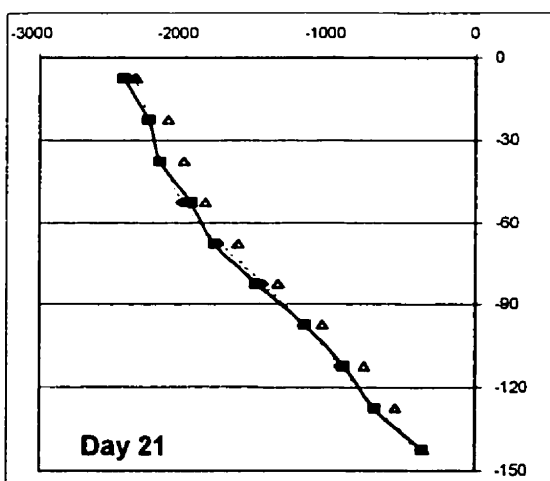
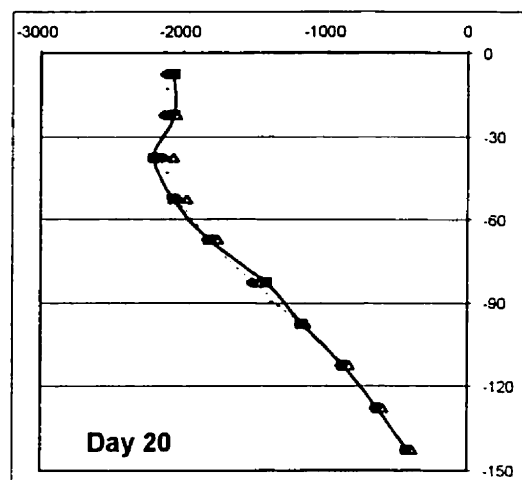
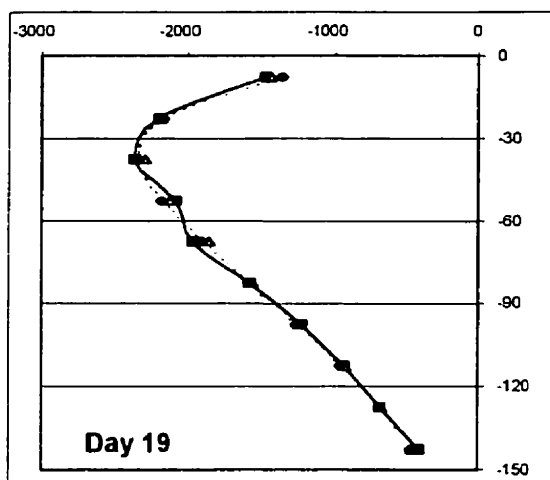
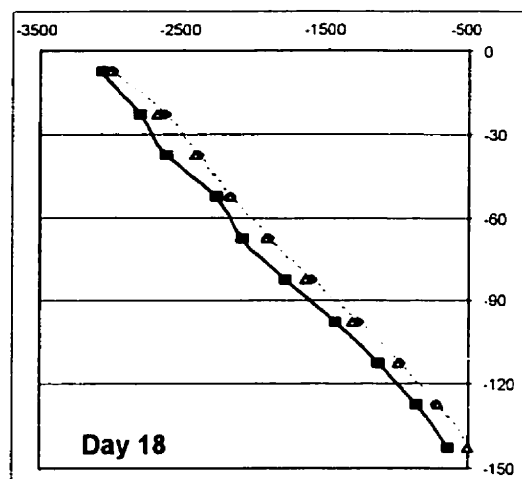
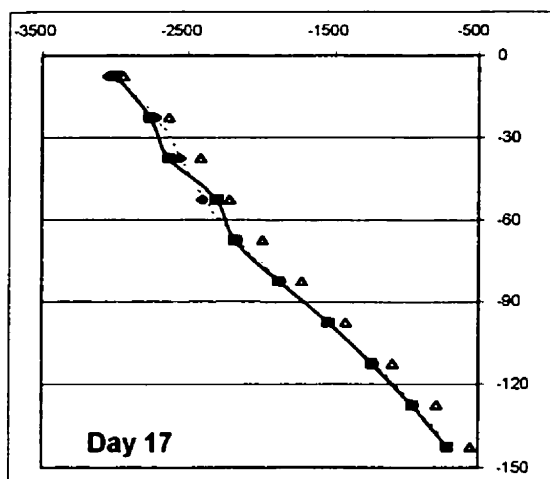


Figure 4.3. Continued

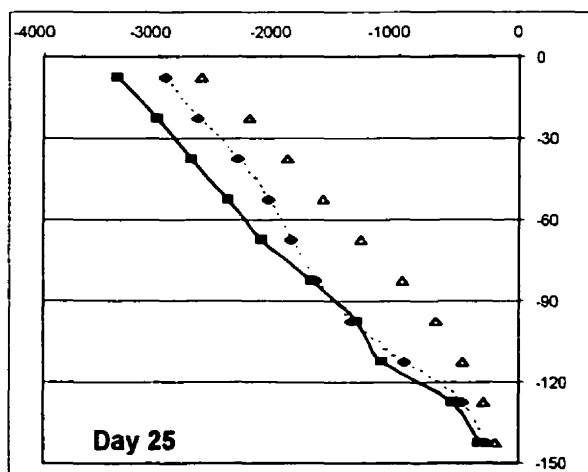
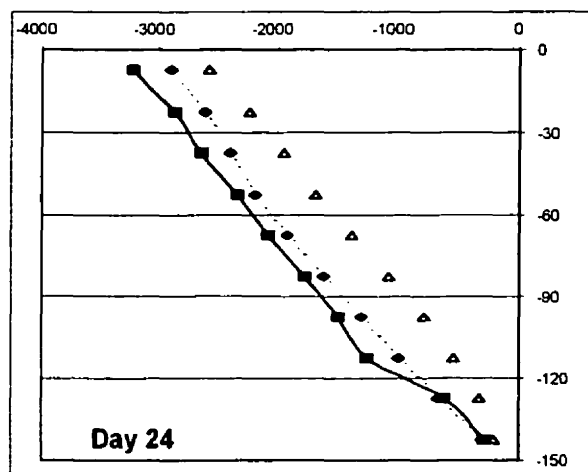
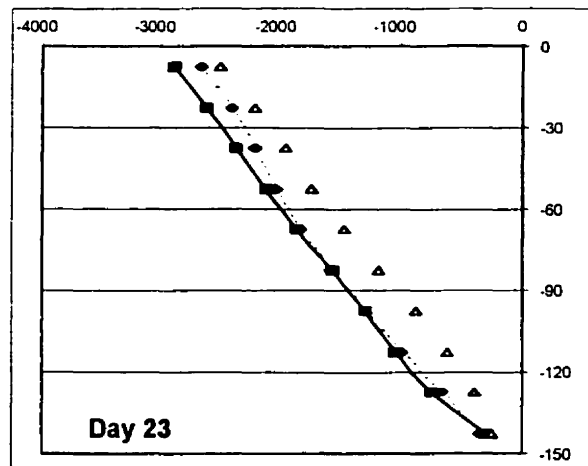


Figure 4.3. Continued

## CONCLUSIONS

VSSM simulation models are expressions of the real world that may explain the reality to a great extent, but not entirely. Moreover, they need to be provided by parameters such as hydraulic conductivity, which are again estimations of real world specifications. ANN learns via examples and is a model-free simulation tool, which helps simulation to get more and more independent of pre-cast models, their limitations, and their parameters. In the lack of real observations, data were generated in this study; however, one of the pros of this approach is that the real world observations can be used to train the ANN. Providing observed records for ANN training incorporates the real world spatio-temporal diversities directly into the model.

Training was cumbersome and time consuming. To find proper ANN structures many trials were done. Preferred ANNs both have three hidden layers and were approved due to their superior performance (Tables 4.1 to 4.6). These ANNs only receive soil-water heads for 10 internal nodes plus some boundary information to estimate new soil-water distribution throughout the soil profile. As a matter of fact, neither hydraulic conductivity nor soil-moisture content is given to the ANNs.

The unsteady ANN-based VSSM flow modeling approach introduced in this paper was capable to mimic the SWAP93 model well. This conclusion may be justified via comparisons provided in Figures (4.2) and (4.3) for sample models M1 and M2. Also, error indicators such as RMS and SCORE were calculated and reported that shows satisfactorily performance of M1 and M2. The execution times for the ANN-based models were almost three times faster than that of SWAP93.

This study bears out the idea that ANN-based models are competent VSSM flow simulators. However, total substitution of a universal ANN-based model instead

of numerical models, needs huge amount of observed data (i.e. a comprehensive / universal VSSM flow database). Such an ANN, which is capable to map all the VSSM flow realities, is a type of huge model-free regression with more individual-data tendency (due to the iterative least square technique used in ANN training) rather than mean tendency. Inasmuch as ANN is sensitive to individual records, it is capable of dealing with real world diversities and data uncertainties. In fact, one of the main motives in employing ANN was to develop a model that has the ability to easily cope with the uncertainty involved in VSSM modeling.

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## **CONNECTING TEXT: CHAPTERS FOUR & FIVE**

This study was planned to be carried out in two parts: 1D, and 3D modeling investigations. The ANN-based approaches developed in the first part are presented in chapters three (ANN-FIS-1D) and four (ANN-1D). The two methods used for ANN inclusion in these 1D models were completely different. ANN-FIS-1D applies ANN in a node-wise manner; i.e., the ANN is trained to estimate a flux only under the influence of a pair of neighboring nodes. However, ANN-1D applies ANN in a profile-wise manner; i.e., the ANN estimates ten nodal soil moisture heads for uniformly distributed nodes across a soil profile.

The second part of the investigation was focused on 3D modeling approaches. In addition to the experience gained in part one, several other ANN inclusion tactics were assessed and eventually one was selected. Chapter five presents a 3D ANN-based approach, ANN-3D, that was developed based on the selected tactic. Also, this chapter presents a 3D simulation model that was tested against the SWMS-3D numerical model.

Inasmuch as the 3D model adopted a node-wise ANN-inclusion tactic, it is in some ways similar to ANN-FIS-1D. Similarities, differences, pros, and cons of the three ANN-based approaches are discussed in chapter 6.

## **CHAPTER FIVE: A 3D NON-NUMERICAL MODEL**

**ABSTRACT:** A three-dimensional non-numerical model for variably saturated soil moisture (VSSM) movement is presented. The model employs artificial neuronet (ANN) techniques to find nodal soil moisture values upon neighboring node soil-moisture values. The Darcy-Buckingham equation was employed to generate data for ANN training. Marching through time and space, the model redistributes soil moisture throughout the flow domain at any time step via recursive excitations of the trained ANN. The ANN, does not require hydraulic conductivity as an input but only the soil moisture content. Two simulation cases were tried, and modeling results were checked with the results of the SWMS model, a three-dimensional model that solves Richards' equation via the finite element approach. Overall good matches were found (SCORE values equal to 93 and 89). Moreover, ANN-based model execution times recorded were three to eight times less than those of SWMS.

### **INTRODUCTION**

A simulation model for Variably Saturated Soil Moisture (VSSM) that is fast and capable of properly handling data uncertainties would serve planners/designers in examining more alternative scenarios to find options that best match their goals. Such a model bestows agricultural/environmental managers the ability to carry out their optimization tasks more comprehensively. Accordingly, development of a simulation model that accepts data uncertainty and lessens computation cost was set as the goal of this study. In this paper, the authors present a simulation model that employs ANN for evaluation of soil moisture variations. The ANN-based approach lowers programming efforts as well as facilitates the preparation of inputs. The model development, as reported in this paper, was based on two pre-modeling steps. Firstly, due to lack of field data, data was generated via Richards' equation. Secondly, an ANN was trained to

estimate soil moisture changes at a node in a three dimensional (3D) space due to the wetness of its six neighboring nodes. Then, a transient 3D model was developed that utilizes the ANN -at any node and any time step- to compute final soil profile moistures. To show how well the new model performed, this paper also presents and discusses the results of two simulation cases using both the ANN-based model and the numerical model, SWMS-3D<sup>5</sup>.

### **NUMERICAL AND NON-NUMERICAL VSSM MODELS**

Almost all existing VSSM-3D flow simulation models are based on numerical solution of the Richards' equation. To develop such models tedious coding effort is needed; however, while employed to simulate natural soil systems high accuracy may not be achieved. This is due to notable uncertainty in the VSSM input parameters, especially for a heterogeneous and non-isotropic 3D flow domain under an undulating soil surface. In fact, 3D simulation results can only be regarded as rough approximations of the real system behavior<sup>1</sup>. 3D-VSSM numerical simulation models are few and are not validated enough to become widely accepted. This is mainly because of two chief obstacles they are faced with: their high computation cost, and data preparation difficulty for their inputs. The computation cost especially magnifies if amply fluctuating boundary conditions and/or sharp moisture gradients occur; both result in the need for several iterations.

To solve the aforementioned problems, a non-numerical approach has been considered as an alternative. The approach introduced in this paper leads to a very lucid code and requires much less execution time compared to that of SWMS-3D. In fact, the proposed non-numeric model has no iterations and utilizes the trained ANN within the entailed ranges for soil moisture variation evaluation. Therefore, its computation is speedy and stable.

The method also has the potential to model real world data directly via ANN training. In fact, ANNs learn directly from examples (i.e. VSSM flow observations), without need for any predefined model. This ability suggests that highly uncertain VSSM flow parameters, such as hydraulic conductivity, may be replaced with some other soil textural and/or structural characteristics that have less inherent variance.

## **MODEL DEVELOPMENT**

The proposed non-numerical VSSM modeling approach has two phases. Phase one deals with training of several ANNs with the objective of defining the structure of the best ANN. Due to the lack of sufficient field observations, data were generated for this study; therefore, phase one is discussed in two parts: data generation and ANN training. Phase two deals with the main model development (that employs the best ANN), henceforth referred to as ANN-3D. To present the approach more pragmatically, a sample model was developed and its performance tested through simulation of two transient VSSM flow cases. The results are presented at the end of this paper, while the succeeding sections give details on modeling stages.

### **Data Generation**

In 3D space every node in a perpendicular mesh system has six neighboring nodes, two on each axis. Any moisture variation in the central node is under the influence of soil moistures in six surrounding nodes. This fact initiates directions about the ANN architecture to be used. Let us name any set of seven nodes, one central and six surroundings, as a Unit Pack (UP). The goal is to estimate final soil moisture for the central node in a UP, when all (seven) initial moisture values are known. To train an ANN that satisfies this goal, data must be generated in a way to provide seven initial soil moisture values as input to the

ANN, and a final (after a certain period of time) soil moisture for the central node as the ANN desired output.

Original soil data for this study were taken from a table in a DRAINMOD reference report<sup>6</sup> that contains soil moisture 'content', 'head', and 'unsaturated hydraulic conductivity' records. To generate data; first, a moisture level was randomly assigned to the central node. Then, soil moistures for neighboring nodes were determined semi-randomly. In other words, to enhance ANN training, one has to consider that the training data set must have a fairly uniform distribution in the universe of possibilities. This may be achieved by defining different moisture classes and assigning moisture contents from these classes at equal frequencies to each node. Then, nodal soil moisture values are assigned by random pick from within the range of each class. Thence, it is called semi-random.

To accomplish the semi-random moisture assignment scheme, the soil moisture range was subdivided into eight arbitrary classes, from very dry to almost saturated. Possible 'moisture class' combinations for each UP (8 moisture classes arranged in 7 nodes) were equal to 8 to the power of 7 (2097152). Moreover, random assignment of moisture contents within each class range creates a huge number of possible 'moisture content' combinations. However, due to computation resource limitations and based on experience/practical applications only 200000 record lines (each with seven volumetric soil contents) were randomly generated by use of a small computer program and considered. Then, the Darcy-Buckingham equation was applied to each record case in order to calculate the flux between the central node and any of the neighboring nodes, assuming a constant mesh spacing of five centimeters. Next, the soil moisture redistribution in the UP under such fluxes for a time period equal to 15 minutes was calculated, leading to the final soil moisture for the central node. At this point each record line has eight data, seven initial values and one final value.

Finally, for the sake of ANN training, records were randomly split into three parts, 50% for training data set, 25% for testing data set, and 25% for verification data set, each saved in separate files.

### **ANN Training**

As discussed above, the ANN architecture for its input (seven initial values) and output (one final value) layers was fixed. However, to find the best ANN internal architecture (i.e. number of hidden layers, number of neurons, and connections) many experiments on several ANN architectures were performed. ANN modules were trained with 'Neural Works Professional II/Plus', version 5.23, software<sup>4</sup>. The 'Extended Delta-Bar-Delta (EDBD) learning rule' and the 'sigmoid transfer function' was found best via trial and errors and used for all neurons. The EDBD learning rule uses past values of the gradient to infer the local curvature of the error surface, and automatically calculates different learning rates and momentum values for each connection. During the ANN training, neuronet 'weights' and overall 'root mean square' (RMS) error for the testing data set were used as training performance indicators to control the process. The ANN training stopped when the testing data set RMS showed no more improvement. Then, the trained ANN was tested against the verification data set via RMS. Note that the RMS values calculated at this stage are for scaled (between 0 and 1, as required by the software) data.

Among all ANN architectures tried, a few were preferred over others due to smaller RMS values based on the scaled data. To find and approve the superior ANN among the preferred ANNs, other error indexes based on unscaled data were checked after training. These error indexes are described below. A structural presentation of the superior ANN, in a linear format, follows: [I(7), H1(7), H2(15), O(1)]\*. In addition to regular connections, the first element in the ANN input layer, which represents initial soil moisture content for the central

ANN input layer, which represents initial soil moisture content for the central node, emits its output not only to the first hidden layer, but also to all 15 neurons in the second hidden layer. Thus, the ANN gives more attention to the information carried by the central node in comparison to other nodes of the UP.

Linear regressions, forced-through-origin ( $Y=b \cdot X$ ) and simple ( $Y=a+b \cdot X$ ), were performed for unscaled data to check the relationship between ANN outputs ( $Y$ ) and desired outputs ( $X$ ). A perfect 1:1 match would have a slope ( $b$ ) equal to one, an intercept ( $a$ ) equal to zero. Also, correlation coefficients, a measure of paired data scattering with a value of one for perfect case, were calculated. Other error indexes based on unscaled data were Mean Absolute Error (MAE) and RMS;

$$MAE = [\sum |D - E|] / n$$

$$RMS = \{[\sum (D - E)^2] / n\}^{0.5}$$

Where,  $D$  and  $E$  are desired and estimated soil moisture heads respectively, and  $n$  is the number of records. In addition, 'SCORE'<sup>3</sup>, a lumped measure of agreement, was also calculated (where 100 is a perfect mach.):

$$SCORE = \{1 - [\sum (D - E)^2 / \sum D^2]^{0.5}\} * 100$$

Values found for these error indicators are reported under results and discussions. After the approval process, the superior ANN was coded as the 'soil moisture estimator' module. At this point phase one was complete and every thing was ready for phase two, model implementation.

### **Model Implementation**

The main model, ANN-3D, computes moisture redistribution through the flow domain. To achieve this, it advances the simulation through space and time while employing the 'soil moisture estimator' module (based on the superior ANN) at any node and at any time step recursively. At each time-step and for each node within the flow domain, a UP is considered. Then, the main program

each node within the flow domain, a UP is considered. Then, the main program to excite the 'soil moisture estimator' module uses known initial soil moistures. Then, the module yields its response, final soil moisture for the UP central node, to the main model. The main model repeats this computation for all nodes for the current time step.

To prevent amplification of errors and to improve model accuracy during simulation, a corrective module was developed that was intended to eliminate imbalances. At the end of each time step, this module calculates the soil moisture balance for the whole flow domain ( $\Delta\text{storage} = \Sigma\text{input} - \Sigma\text{output}$ ). Then, it checks for minor errors and corrects the imbalances, if there were any. The corrective measure assumes that the final 'soil moisture distribution pattern' is correct. To abolish the imbalance quantity, it is distributed to all nodes, not uniformly, but conforming to the soil moisture pattern. For instance a wet node receives a large corrective share, whereas a dry node receives a small one.

In more detail, the ANN-3D model performs several estimations, each from a UP 'initial condition' and the ANN output is the 'final condition' for the central node. Initial and final conditions are in terms of soil moisture ( $\theta$ ); therefore, the first step was to find initial and final soil moisture heads ( $h$ ) for boundary nodes. The next step is to find initial and final boundary fluxes and overall boundary flow (Moisture Inputs - Moisture Outputs) for the current time step. Total initial and final soil moistures content/storage were also calculated. As a result, one may employ the soil profile balance equation to find the Total Moisture Correction (TMC) as follow:

$$\mathbf{TMC} = (\text{Moisture inputs} - \text{Moisture outputs}) - (\text{Change in moisture storage})$$

$$\mathbf{TMC} = (\text{Bottom flow} + \text{Top flow} + \text{Lateral flow}) - (\text{Final storage} - \text{Initial storage})$$

Note that negative or positive signs in TMC denote a need to decrease or increase the final soil-moistures, respectively. The next step was to use the soil-moisture



moisture contents ( $\theta_i^*$ ). This was done via corrective coefficients (= the ratio of 'nodal moisture' / 'total moisture') multiplied by TMC, as shown below:

$$\theta_i^* = \theta_i + [(\theta_i / \Sigma \theta_i) * TMC]$$

With the ANN-3D model in hand, two transient cases were simulated, named as Run-1 and Run-2, with ANN-3D and SWMS-3D. The ANN-3D outputs were tested against those of the SWMS-3D good matches were found. The SWMS-3D model numerically solves the Richards' equation for saturated-unsaturated water flow and the convection-dispersion equation for solute transport. The governing flow and transport equations are solved numerically using Galerkin-type linear finite element schemes.

The results are presented and discussed in the next section. The flow domain dimension, initial conditions, and boundary conditions for both simulations follow. Note that Z is defined as zero at the bottom of the flow domain, and maximum at the top or soil surface.

#### **Run-1.**

Flow domain dimensions:       $X = 10 \text{ cm};$        $Y = 10 \text{ cm};$        $Z = 250 \text{ cm};$

Initial conditions ( $t = 0$ ):

$h = -150 \text{ cm};$       for all  $X, Y,$  &  $Z$

Boundary conditions ( $t > 0$ ):

$dh/dZ = 0$  (Free drainage);      for  $Z = 0 \text{ cm}$ , all  $X$  &  $Y$ ;

$dh/dX = 0$  (no lateral flux);      for  $X = 0 \text{ cm}$  or  $X = 10$ , all  $Y$  &  $Z$ ;

$dh/dY = 0$  (no lateral flux);      for  $Y = 0 \text{ cm}$  or  $Y = 10$ , all  $X$  &  $Z$ ;

$h = -2500 \text{ cm};$       for  $Z = 250 \text{ cm}$ , all  $X$  &  $Y$ ;

#### **Run-2.**

Flow domain dimensions:       $X = 50 \text{ cm};$        $Y = 50 \text{ cm};$        $Z = 250 \text{ cm};$

Initial conditions ( $t = 0$ ):

$h = -150 \text{ cm};$       for all  $X, Y,$  and  $Z$

Boundary conditions ( $t > 0$ ):

$dh/dZ = 0$ (Free drainage);	for $Z = 0$ cm, all $X$ & $Y$ ;
$dh/dX = 0$ (no lateral flux);	for $X = 0$ cm or $X = 50$ , all $Y$ & $Z$ ;
$dh/dY = 0$ (no lateral flux);	for $Y = 0$ cm or $Y = 50$ , all $X$ & $Z$ ;
$h = -2500$ cm;	for $Z = 250$ cm, $X = 0$ , all $Y$ ;
$h = -2300$ cm;	for $Z = 250$ cm, $X = 5$ , all $Y$ ;
$h = -2100$ cm;	for $Z = 250$ cm, $X = 10$ , all $Y$ ;
$h = -1900$ cm;	for $Z = 250$ cm, $X = 15$ , all $Y$ ;
$h = -1700$ cm;	for $Z = 250$ cm, $X = 20$ , all $Y$ ;
$h = -1500$ cm;	for $Z = 250$ cm, $X = 25$ , all $Y$ ;
$h = -1300$ cm;	for $Z = 250$ cm, $X = 30$ , all $Y$ ;
$h = -1100$ cm;	for $Z = 250$ cm, $X = 35$ , all $Y$ ;
$h = -900$ cm;	for $Z = 250$ cm, $X = 40$ , all $Y$ ;
$h = -700$ cm;	for $Z = 250$ cm, $X = 45$ , all $Y$ ;
$h = -500$ cm;	for $Z = 250$ cm, $X = 50$ , all $Y$ ;

## RESULTS AND DISCUSSION

The ANN-3D model is based on an ANN which excites via seven 'initial soil moistures' of a UP, and estimates the 'final soil moisture' for the UP central node.

**Table 5.1.** Performance indicators of the superior ANN, based on the three data sets used. Perfect values for these indicators are reported in the first row.

	<b>a</b>	<b>b</b>	<b>b'</b>	<b>R</b>	<b>RMS</b>	<b>MAE</b>	<b>SCORE</b>
Perfect value	0.0	1.0	1.0	1.0	0.0	0.0	100
Training	0.03725	0.9128	0.9963	0.9561	0.02309	0.01694	94.74
Testing	0.01802	0.9215	0.9969	0.9588	0.02244	0.01643	95.36
Verification	0.03561	0.9097	0.9952	0.9556	0.02351	0.01721	94.73

The superior ANN, [I(7), H1(7), H2(15), O(1)], achieved an RMS value equal to 0.0032 (for scaled data). As mentioned earlier, the unscaled ANN outputs were also verified in detail with SCORE, RMS, MAE, correlation coefficient, and regression lines ( $[E = a + b * D]$ , and forced-through-origin  $[E = b' * D]$ ) slopes

and intercept. These indicators are reported in Table (5.1) for training, testing, and verification data sets. Perfect values for all indicators is given in the first row. As the indicators in the table show, the ANN performance is quite acceptable.

The initial plan for ANN training was to train and employ an ANN that estimates soil-moisture heads. However, due to high variation in the range of soil moisture heads (with differences of up to four orders of magnitude) and the huge number of possible combinations, training trials failed to bring forth an appropriate ANN. In fact, training tasks for this study were tedious and time consuming. Obviously, in comparison to a 1D flow domain (each UP has only three nodes), for a 3D case (with seven nodes in each UP) complexity of the problem increases drastically. On the other hand, despite the hypothetical belief that ANNs are universal estimators and are theoretically capable of achieving zero error, for most cases it is practically impossible to train an error-free ANN. Therefore, an amendment was necessary. Then, instead of using 'soil moisture head' data the feasible solution adopted was to use 'soil moisture content' data. The advantage is that ANN training would be faster due to the smaller range of variation of soil moisture contents (with only one order of magnitude). However, a disadvantage is the inability of such an ANN to solve saturated flow problems. In other word, when ANN receives its inputs in terms of 'soil moisture content', it fails to reflect soil water head variabilities in a saturated medium.

As aforementioned, the overall performance of the ANN-3D model was tested against the SWMS-3D model through two illustrative simulation cases, Run-1 and Run-2, each for a 25 day simulation period. Flow domain dimensions, initial conditions, and boundary conditions for both runs are introduced above. Results of both runs are presented separately and then discussed together below.

Run-1 was designed as a 1D vertical flow in a 3D flow domain. This provides an easy way to visualize the results of both models, which in turn, helps us to

Run-1 was designed as a 1D vertical flow in a 3D flow domain. This provides an easy way to visualize the results of both models, which in turn, helps us to compare and contrast the results in more detail. The results for Run-1 simulation case are presented in Figure (5.1) which includes 12 graphs for selected days. The graphs compare results of simulations performed by both (ANN-3D, and SWMS-3D) models, and visualize continuous moisture alterations along the flow domain depth (Z axis). Assuming SWMS-3D results as observed values (i.e. desired outputs), RMS and SCORE for ANN-3D were calculated and found equal to 220.71 and 93.05 for the first case simulated, which interprets as a good match. Relative errors for individual data points range from 0% to 35%, with an average of 14.69% and a standard deviation of 7.82%.

Run-2 was designed as a 2D flow (X-Z plane) in a 3D flow domain. Results of this run, as presented in Figure (5.2), are presented as contour graphs of soil moisture heads in the X-Z plane. To compare and contrast results of both (ANN-3D and SWMS-3D) models, while tracking continuous moisture alterations through the simulation period, Figure (5.2) presents four contour graphs for selected days. In the same fashion as before, SWMS-3D results were assumed as observed values (i.e. desired outputs). Thereupon, RMS and SCORE for ANN-3D were calculated to be 131.04 and 89.05 for this case simulated, which denotes a good match. Relative errors for individual data points range from 0% to 54%, with an average of 11.32% and a standard deviation of 12.04%.

In order to be compared with SWMS-3D results, ANN-3D outputs were turned into soil moisture head values via interpolation between tabulated data. From the Run-1 and Run-2 results graphed in Figures (5.1) and (5.2), several points may be made. First of all, an over all good mach is attained in both cases. ANN-3D results are, in general, compliance with SWMS-3D results, and follow the same trend. However, as the simulation proceeds, some local disagreements magnify, which are more intense in the case of Run-2. This may be the result of

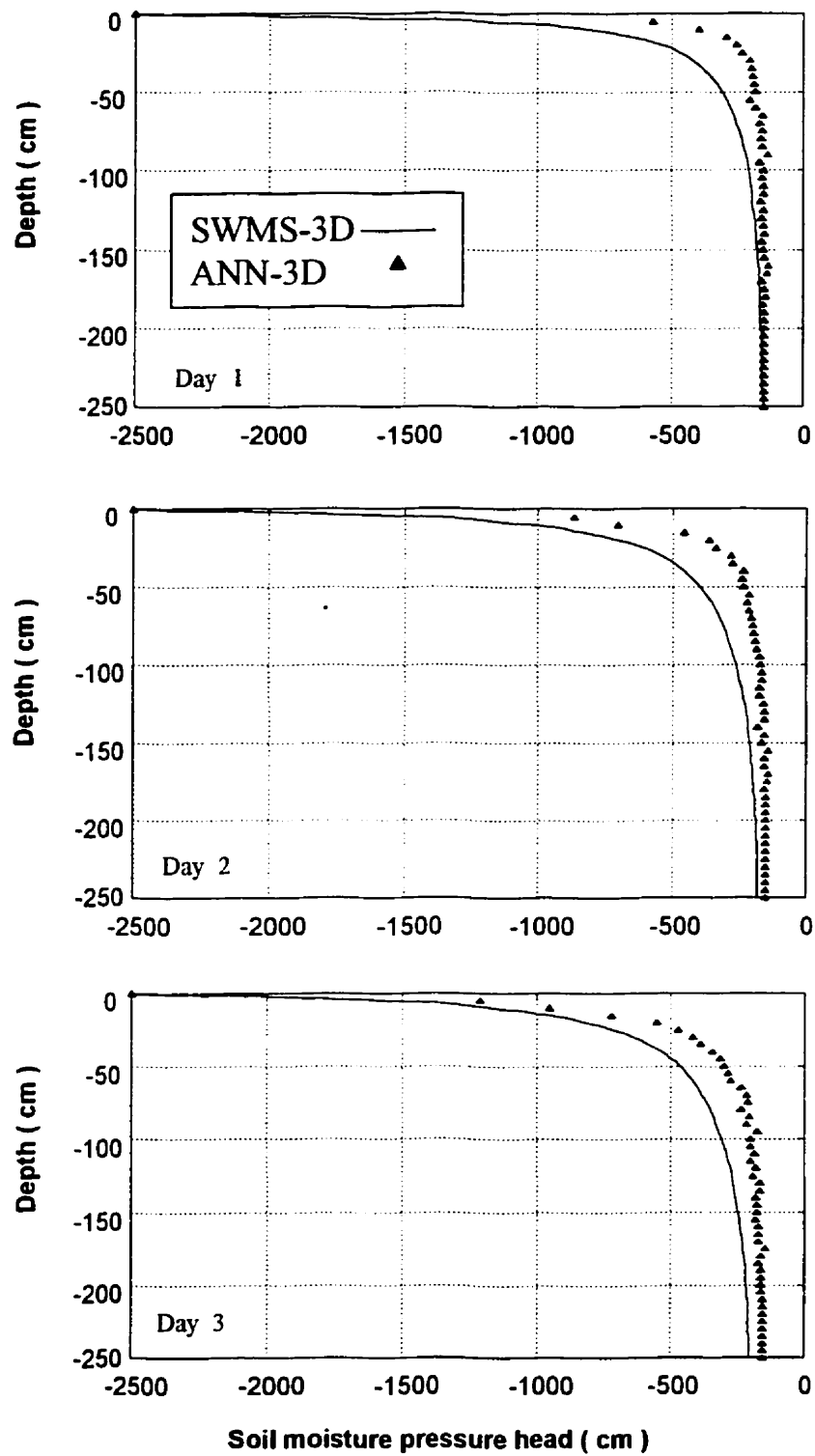


Figure 5.1. Some plotted results for the first simulated case.

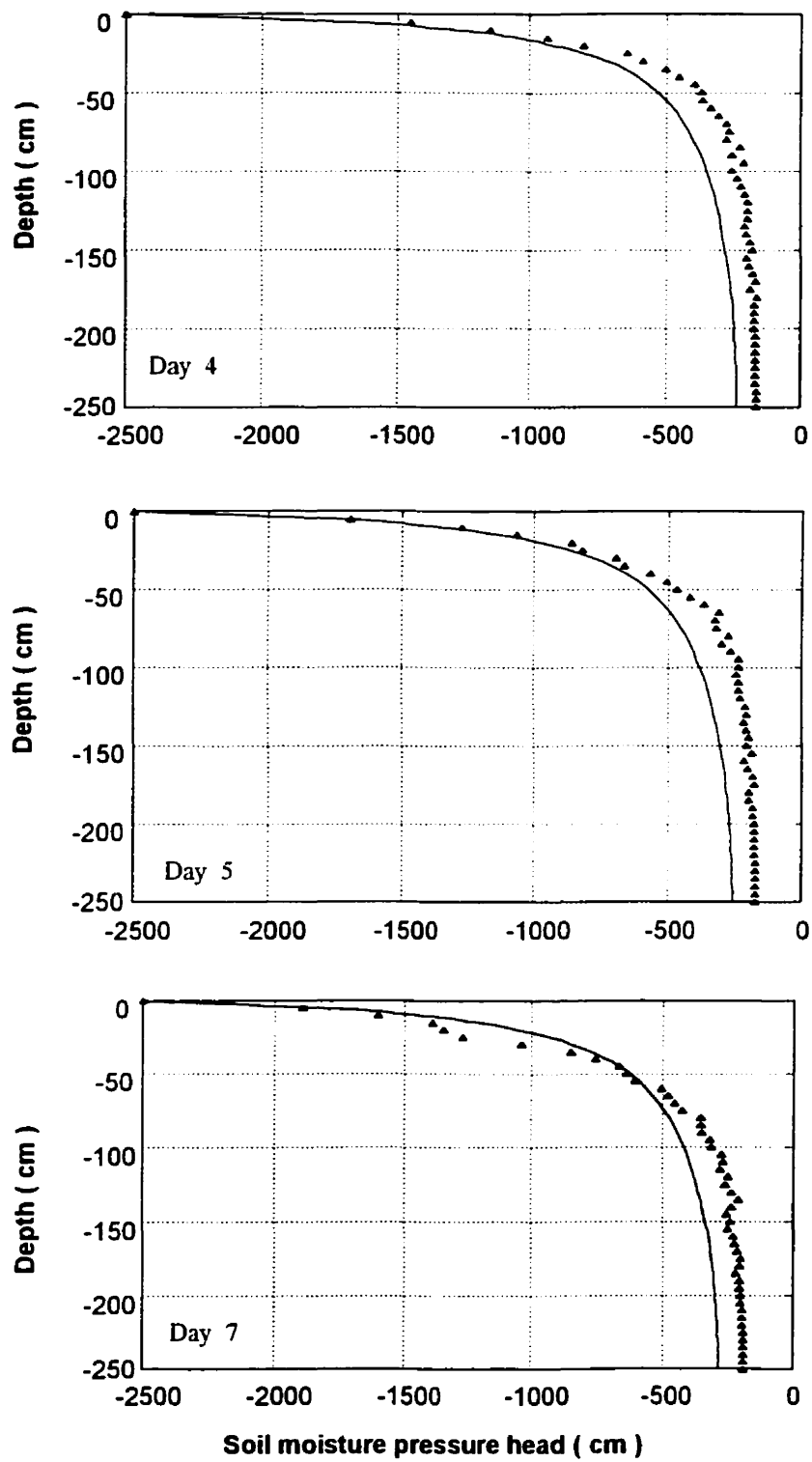


Figure 5.1. Continued.

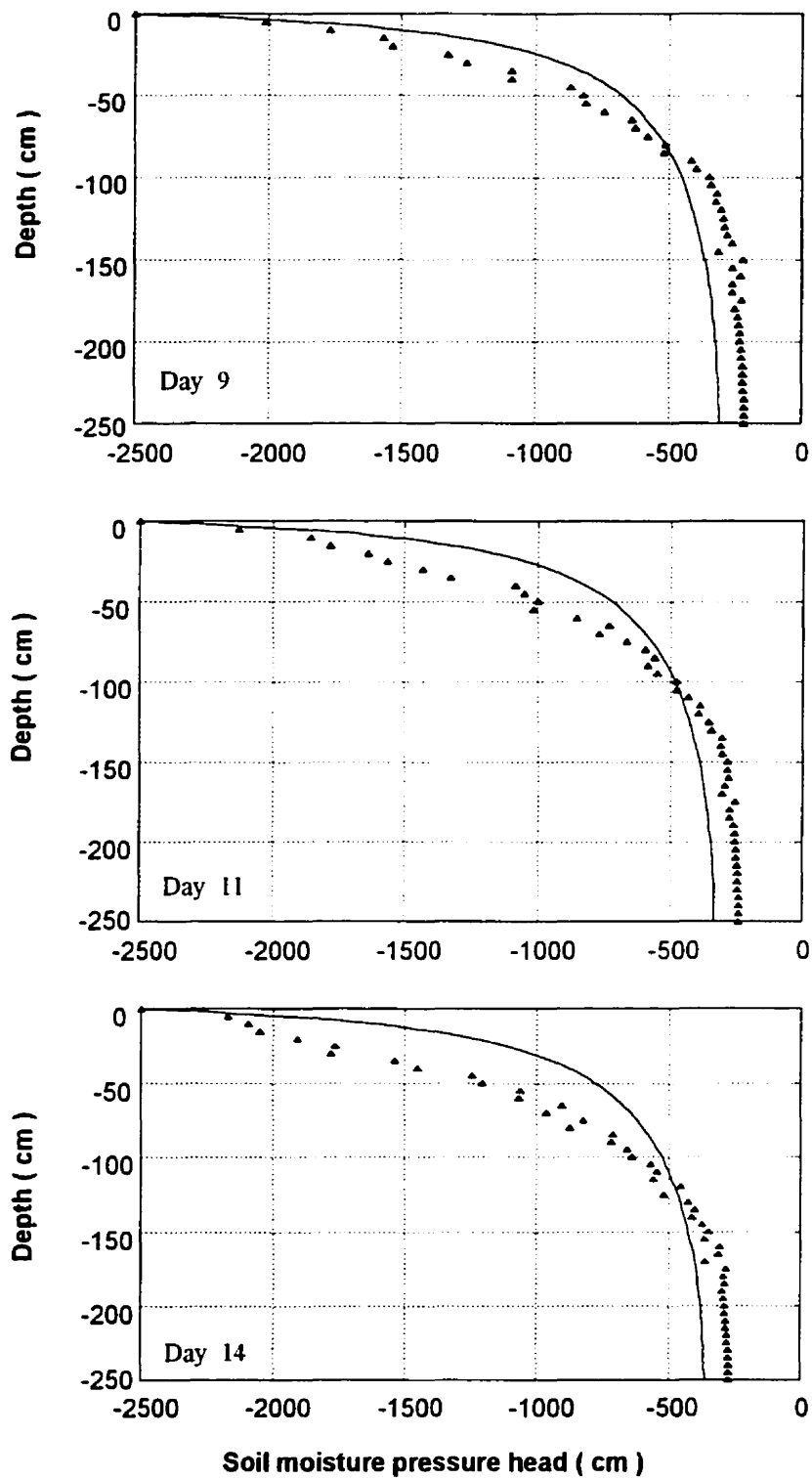


Figure 5.1. Continued.

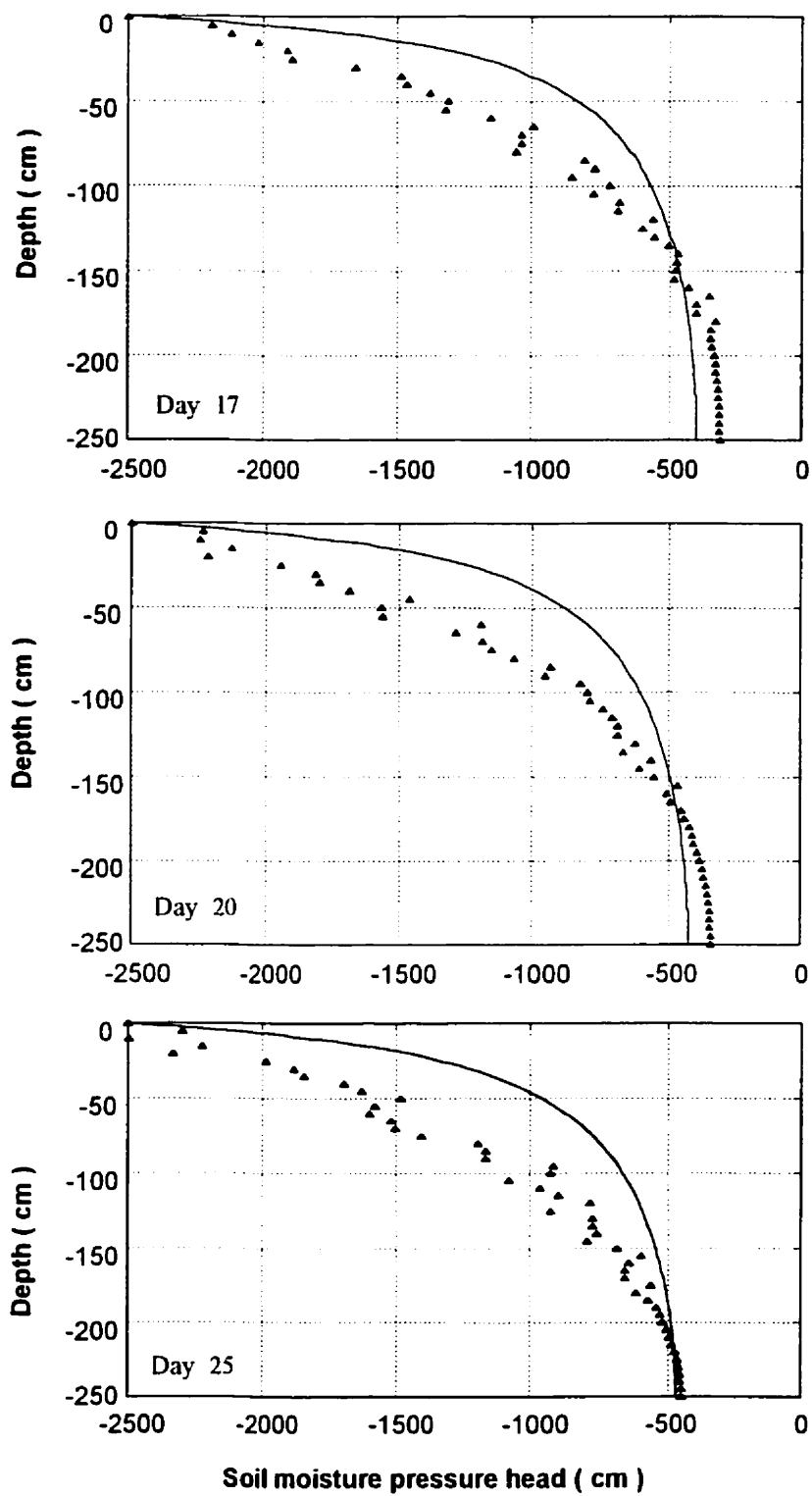


Figure 5.1. Continued.



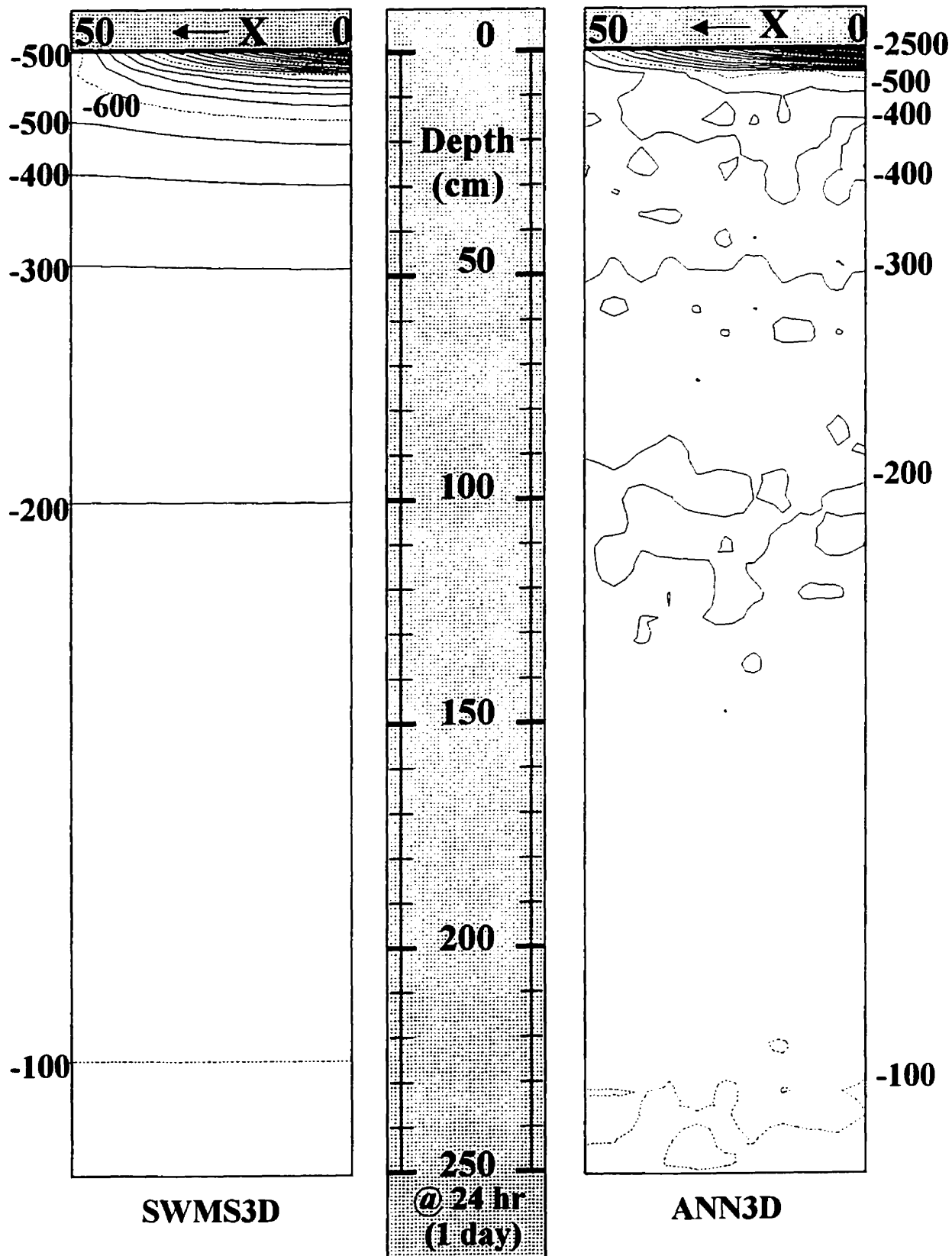


Figure 5.2. Contour plots for the second simulated case.

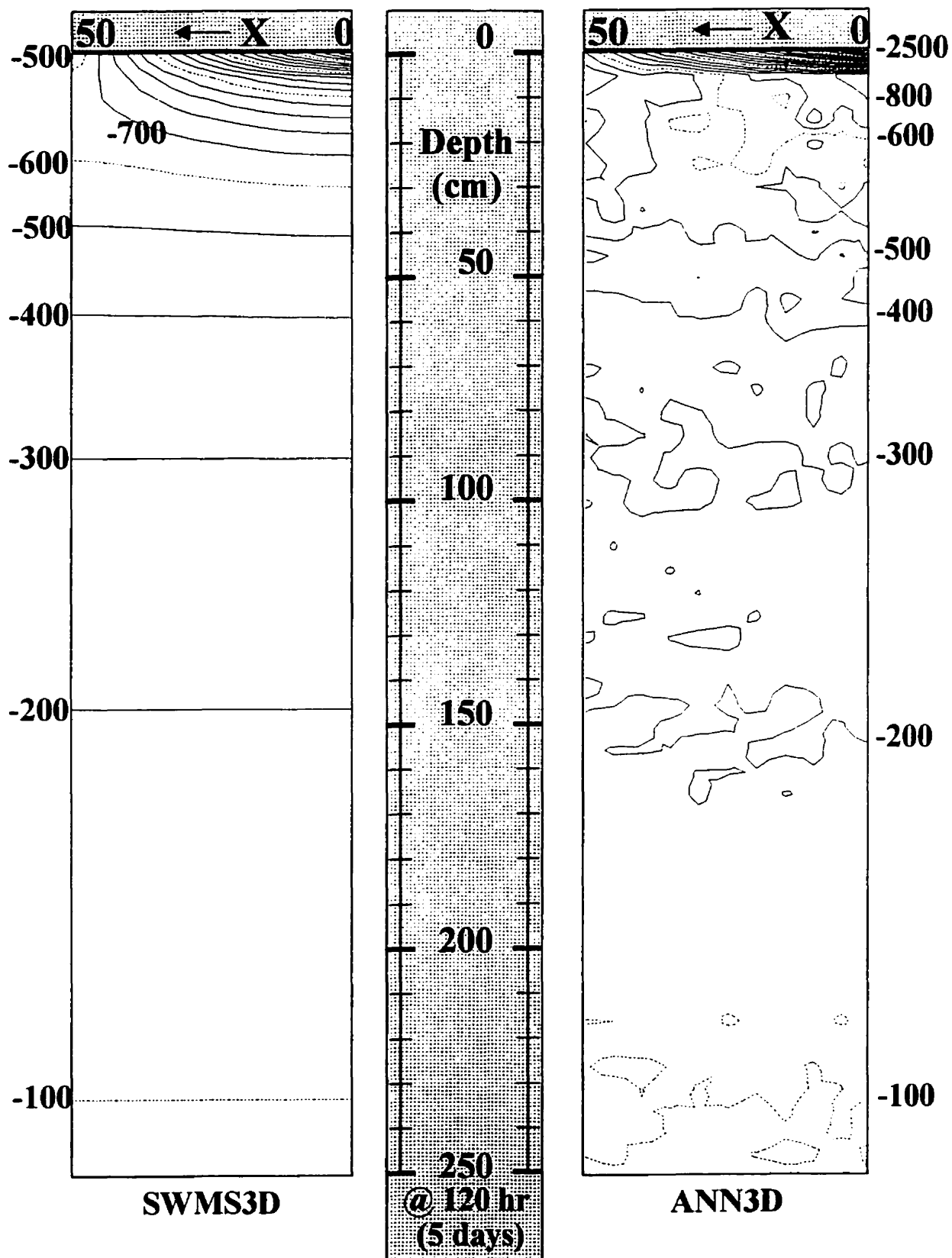


Figure 5.2. Continued.

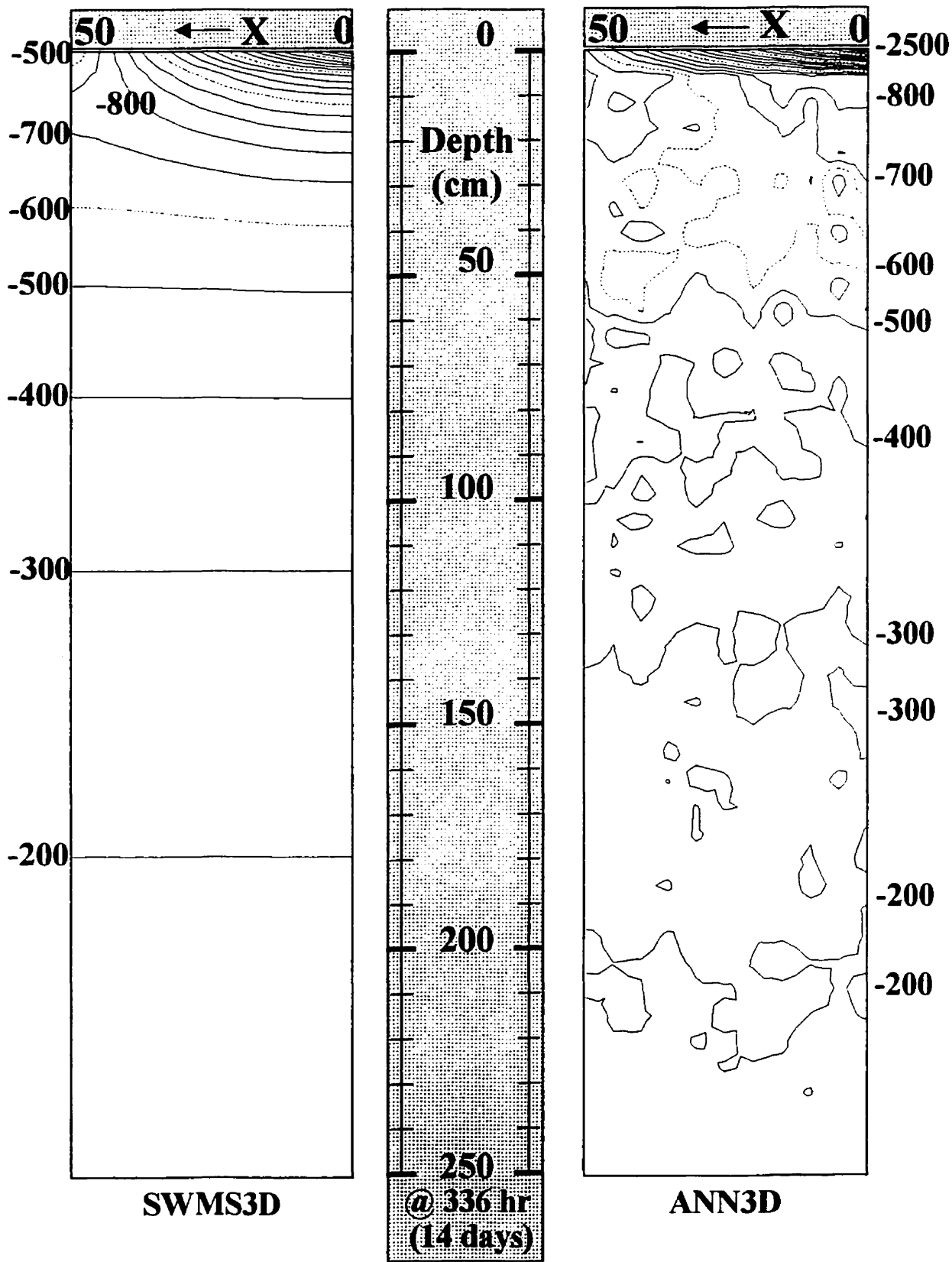


Figure 5.2. Continued.

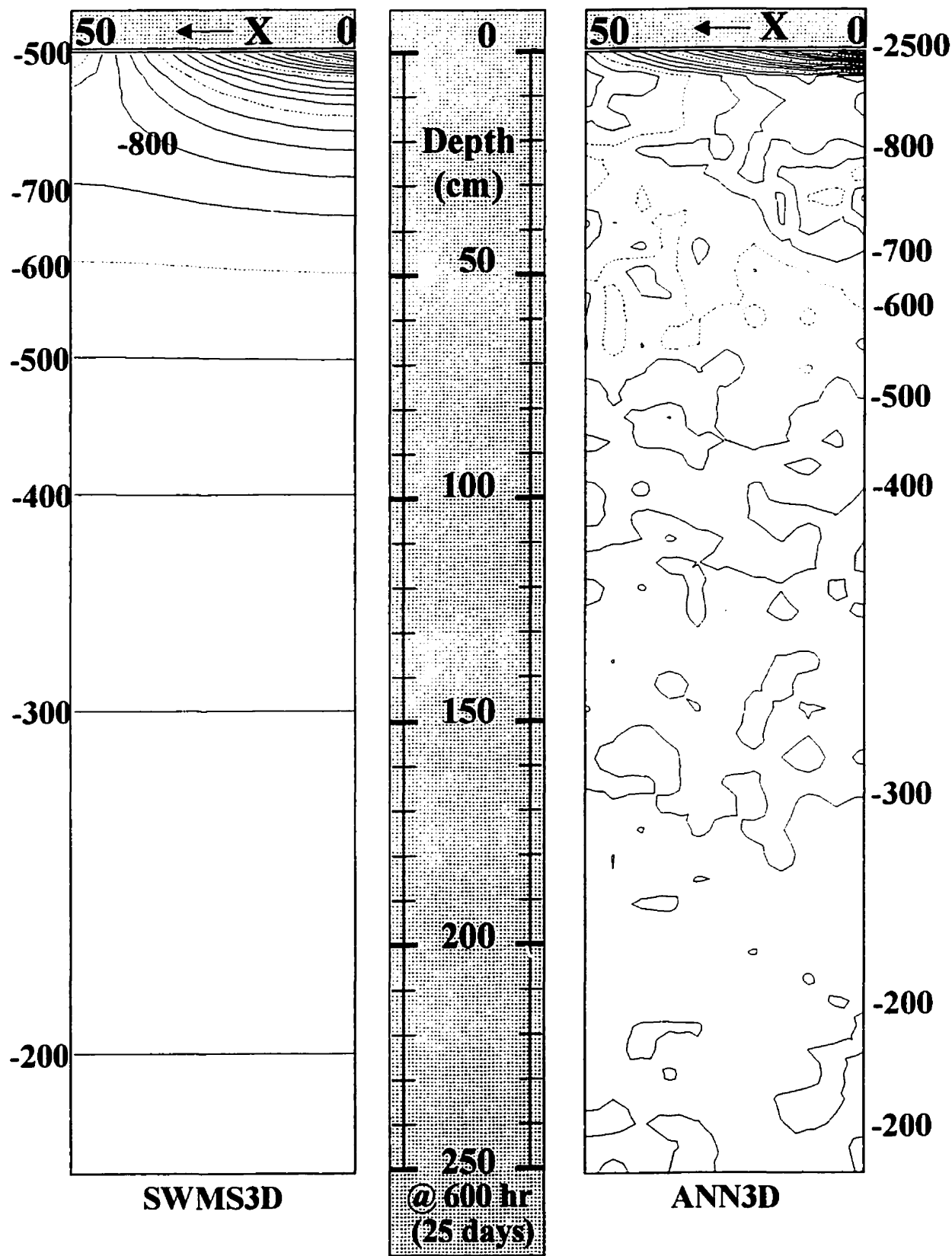


Figure 5.2. Continued.

Another noteworthy point is the minor randomness seen in the ANN-3D results. This is evident in the form of the scattered data points in Run-1 graphs, and in the form of closed pockets and rough irregular contour lines in Run-2 graphs. Worth noting is that supervised back-propagation ANN training is a data driven model (not a mechanistic one) that may be referred to as a 'superior regression technique'. Therefore, these random deviations may be described as a direct result of the ANN generalization, just in the same way as regression averaging. Also, it has to be mentioned that collected data from a real field soil profile, if plotted, has little likelihood of exhibiting smooth lines, such as those in the SWMS-3D graphs. Moreover, when real world data (with high variance and a serious noise level) are of interest, the fact that ANN generalization is beneficial should not be overlooked.

Finally, execution times for both models were recorded. Simulation models, ANN-3D and SWMS-3D, were executed on a PC platform with P-III processor at 600 MHz. The ANN-3D model execution times were 47.41 and 385.33 seconds, with 200 and 5000 nodes, for Run-1 and Run-2 respectively. The SWMS-3D model execution times were 143 and 3237 seconds, with 720 and 8349 nodes, for Run-1 and Run-2 respectively. Comparison of these timings show three to eight times shorter execution times for the ANN-3D model. These results may be affirmed by the fact that the number of computation steps for the ANN-3D model were much less than those needed for the SWMS-3D model.

## **CONCLUSIONS AND RECOMENDATIONS**

Customary 3D VSSM simulation models are based on numerical solution of Richards' equation. High computation costs and the need of detailed data input of these models are the most important drawback factors against their popularization. Moreover, the parameters used, such as hydraulic conductivity, generally have an inherently large variance. Measurement of these parameters requires substantial time and money. This study was aimed at exploring an

ANN-based alternative approach to these routine numerical simulation practices, and to determine its feasibility in terms of veracity, computation cost, and input facilitation.

Our interest in the ANN approach emanates from the fact that it learns from examples and is a data-driven simulation tool capable of mimicking complex patterns. This provides a direct link between real world observations and modeling. This renders the possibility to adopt complexities of a real system by a model. Further, ANN is a model-free simulation tool, which helps to minimize dependence upon pre-cast algorithms and their rigid parameters. This study, faced with the lack of real observations, did not have the chance to demonstrate a direct link between real world observations and the model. However, it was shown that the ANN approach is quite capable of such an advantage.

Veracity of the ANN-3D was checked against the SWMS-3D model. Results show a good general match; however, relative errors for individual data (nodal soil moisture values) were as high as 54%. Generally speaking, results show the ability of the new approach to model the VSSM flow. However, much has yet to be done to attain an ANN-based model with general applicability and higher veracity. Future works on this issue are needed in two ways. First, collection of real world data to form a universal 'VSSM redistribution' database. In fact, such a database, which implicitly contains descriptions of highly non-linear VSSM redistribution phenomenon, would be a treasure for VSSM modelers that might be used in several other ways. Second, development of ANN training methods, which are faster and better (i.e. able to find the global minimum error on rough multi-dimensional error surfaces). A drawback of the 'soil moisture estimator' ANN-based module was that it did not heed preservation of mass. With a better ANN training method, it seems possible to incorporate mass balance as a factor in ANN training as well. Another disadvantage was the long time and tedious efforts needed to train ANNs and find the best ANN for nonlinear cases such as

VSSM redistribution, even for a small data set as used in this study. A faster ANN training approach is a real need for any further work in this domain. Otherwise, the time and effort needed to train an ANN, as 'universal VSSM redistribution estimator' will be a serious barrier.

ANN-3D computation costs for both simulated cases were significantly lower than those of SWMS-3D. The size of the ANN structure is very influential with respect to computation cost. Smaller or larger ANNs can directly decrease or increase the model computation costs, respectively. Introduction of more data sets (with different soil types) increases the number of inputs and complexity. This in turn means a larger ANN size, which deteriorates the ANN-3D superiority in computation cost. A cure to this is possible through application of many ANNs, each specially trained for different cases and therefore having a smaller structure. These could then be connected via a FIS (Fuzzy Inference System) to simulate VSSM redistribution. Any attempt to keep the ANN size minimal would increase the speed of computation.

The 'soil moisture estimator' ANN-based module does not need hydraulic conductivity values for VSSM redistribution calculations. In fact, using only one soil type gives ANN the chance to implicitly capture information, as a function of soil moisture from soil moisture data. If more soil types are to be considered, then instead of hydraulic conductivity, some soil textural and structural data (soft/qualitative or hard/quantitative) might be used to pass the information on to the ANN. This is a great advantage because elimination of such highly variable parameters, such as hydraulic conductivity, saves time and money. Furthermore, this would allow the model to find out more information about the real system. That is, the model receives core information before being masked by predefined models and their parameters.

Overall, this study showed that the ANN-3D approach is a potential VSSM redistribution simulation method. The method has a more lucid code, requires

less execution time, needs fewer and more basic inputs, and is capable of handling the uncertainty involved in VSSM modeling. However, there is a lot more to be done before total substitution of numerical models is possible with ANN-based models.



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## **CHAPTER SIX: GENERAL SUMMARY AND CONCLUSIONS**

This study was an investigation on applicability of Artificial NeuroNet (ANN) and Fuzzy Inference System (FIS) techniques for 'simulation modeling of Variably Saturated Soil Moisture (VSSM) redistribution', a main component of Soil Hydrology Processes (SHP). This chapter presents four separate sections on various topics to provide a general view of the study performance. The study summary is given in the first section. The second section compares the three simulation models developed in this study in order to highlight pros and cons of each approach adopted. Next, the third section draws some general conclusions based on the whole context of the study. At the end, the fourth section contains some remarks on potential practical benefits of application of ANN and FIS techniques for simulation modeling of VSSM redistribution.

### **SUMMARY**

Existing VSSM simulation modeling approaches were reviewed in Chapter two. The review emphasized alternative approaches to conventional numerical approaches. SHP models may be classified in many ways, such as: discrete versus continuous, steady versus unsteady (transient), one- or two- or three-dimensional, and research versus practice-oriented. In a general classification, described at the end of chapter two, physical (including 'analog' and 'replica') and non-physical (also called 'abstract' or 'conceptual') models were taken as known root level classes. Non-physical modeling may be done via different means such as equations, graphs, databases or tables, rules, and linguistic knowledge bases. Models in this category were classified from four different points of view.

The first point of view classifies non-physical models in two sub-classes: 'black-box' versus 'white-box' and 'gray-box'. Models in the latter case are based on phenomenal explanations and include most SHP non-physical models. Black-box

models such as regression and ANN techniques, model the relationship between inputs and outputs blindly; and are favorable for very complex phenomena which are not comprehended, nor yet explained.

From the second point of view, non-physical models were categorized in two sub-classes: 'mathematical' (including 'analytical' and 'numerical') versus 'non-mathematical'. Inasmuch as computers are based on binary digits, conventional SHP simulation models have been based on mathematical expressions that only accept numeric (hard) data. Recent innovations in computer technology have, somewhat, enabled computer simulation models to handle non-numeric (soft) information as inputs and/or outputs.

Thirdly, non-physical models were grouped into 'deterministic' versus 'non-deterministic' models. Field soil heterogeneity has restricted the application of deterministic models mostly to very small-scale problems. The 'effective parameter' concept was developed as a solution to the scale barrier. But, in the presence of high field heterogeneity and random sources of data variation, uncertainty has to be considered by non-deterministic modeling. Stochastic models, the traditional non-deterministic modeling approach, has been in practice during the last three decades and resolve the scale barrier statistically. Alternatively, novel non-deterministic approaches employ artificial intelligence techniques as data uncertainty handling tools.

The fourth point of view classifies SHP models into 'empirical' or 'data driven' versus 'mechanistic' models. As much as a model considers physics of the process to model, it becomes more mechanistic and independent of data. Two extreme sides of this classification are 'fully mechanistic' (pure white box) and 'fully data driven' (pure black box) models.

Most conventional SHP models can be classified as deterministic-mathematical(-numerical)-mechanistic. In recent years due to new opportunities provided,

alternative models (non-deterministic and non-numerical) have gradually emerged in SHP modeling. For example, use of fuzzy variables in VSSM modeling has provided the chance to employ soft data. Also, use of ANNs has opened a way to model highly complex and non-linear relationships with reasonable error even when data is uncertain and noisy. ANNs are data driven models that theoretically have the powerful capability of being universal function approximation tool. Hence, they are best suited for modeling of VSSM redistribution. However, to find proper ANN structures many training trials, each cumbersome and time consuming, have to be done.

The strategic idea in the background of this study was based on the usage of ANN in place of Richards' equation as the heart of the model. Inasmuch as Richards' equation was originally derived from "Darcy-Buckingham" and "continuity" equations, it is subject to the Darcy equation limitations. Therefore, Richards' equation does not count for other forms of flow other than Darcian flow, such as preferential flow and osmotic induced flow. Traditionally, VSSM flow numerical models, based on Richards' equation, utilize other equations for these additional circumstances. However, the ANN model can overcome such limitations, if trained with a comprehensive set of field data including information on macro-pores, salinity, ... etc.

Chapter three gives brief introductions to ANN and FIS techniques, followed by a complete report on the development of the first 1D VSSM redistribution simulation model (ANN-FIS-1D). To minimize the ANN approximation error on the highly non-linear VSSM flow, usage of multiple ANNs was adopted. In total 25 ANNs were trained, each for one of 25 fuzzy classes of flux. Consequently, to fulfill the need for integration of the ANNs outputs, FIS came into the framework. The ANN does not require hydraulic conductivity as input. The model was tested against SWAP93 with a maximum error of less than eight percent. This satisfactory result demonstrates the capability of the ANN-FIS-1D approach in simulation of

VSSM redistribution. The tactical method used for integrating ANN into the ANN-FIS-1D model was 'binodal'; i.e., ANN estimates the flux between 'two adjacent nodes' each time it is referred to by the simulation model.

Chapter four is dedicated to report on the development of the second 1D VSSM redistribution model (ANN-1D). While the strategy was the same as before, two tactical methods adopted were largely different from the one explained above. In both of these methods ANNs receive excitements from the simulation model as ten soil moisture heads (of ten internal nodes spaced uniformly across the soil profile), plus boundary conditions for last and current times. The ANNs responses, however, were different. The first one estimates 'the soil moisture heads for ten nodes uniformly spaced across the soil profile' and the other estimates 'the six coefficients of a fifth degree polynomial'. This model also does not need hydraulic conductivity as input. The unsteady ANN-1D approach introduced in chapter four was able to mimic the SWAP93 model well. This conclusion may be justified by reviewing error indicators reported. The recorded execution times for the ANN-1D models were almost three times faster than that of SWAP93.

The ANN-3D model development is reported in chapter five. The way ANN was integrated into this model in essence follows the way adopted by the ANN-FIS-1D model (i.e, nodal); however they have many practical differences. At each time step and for each node within the flow domain, ANN receives seven initial 'soil moisture contents' and estimates one final soil moisture content. The set of seven nodes are defined as a central node and six neighboring nodes in 3D space (two on each axis). Veracity of the ANN-3D was checked against the SWMS-3D model. Results show a good general match. Moreover, the recorded execution times show a three to eight times decrease for the ANN-3D compared to the SWMS-3D model.

Overall, this study showed that the ANN-based approaches are potential VSSM redistribution simulation methods. These methods have more lucid code, require less execution time, need fewer basic inputs, and are capable of handling the uncertainty involved in VSSM modeling.

### **COMPARISON OF THE ANN-BASED MODELING APPROACHES**

This section compares and contrasts the three ANN-based simulation approaches developed in this study. To do so, emphasis is given to: ANN inclusion tactic, computation costs, and simplicity of the input data requirements of these approaches.

Overall, four different ANN inclusion tactics were adopted in this study, where hydraulic conductivity was not required by any of these ANNs as an input. However, the sequences and types of inputs and outputs are different for each of these ANNs.

The most simple ANNs were the two (M1 and M2) used in the ANN-1D models, as described in chapter four. The M1 structure in linear format is [I(17), H1(3), H2(10), H3(10), O(10)]; and for M2 is [I(17), H1(12), H2(10), H3(8), O(6)]. The ANNs were trained for a fixed time step equal to one day (24 hours). Their input vector includes the soil profile depth, ten initial soil moisture heads, and information on upper and lower boundary conditions for the current time (t) as well as for one day before (t-1, initial state). The ANN used by M1 estimates ten soil moisture heads for uniformly distributed nodes within the soil profile. However, the other ANN (used by M2) predicts six coefficients of a fifth degree polynomial that demonstrates a relationship between 'soil profile depth' and 'soil moisture head'. In fact, the polynomial provides access to known soil moisture heads at any soil profile depth. Both ANN structures are large when compared with the other ANNs, but the computation cost is very small which is

due to the large time step and the fact that for each time step the ANN is excited only once to renew the soil profile heads.

Both of the subsequent tactics used are different from the one discussed above in that they only solve the problem for a single node (not the whole soil profile). Therefore, the main program has to send several pulses (equal to the number of nodes defined in the soil profile) to excite these ANNs for each time step.

The ANNs employed in ANN-FIS-1D as explained in chapter three all have similar structures as may be expressed in linear format as  $[I(2), H1(5), H2(3), O(1)]$ . They receive input vectors with only two soil moisture heads that represent a pair of adjacent nodes within the soil profile. Then, the ANNs approximate the steady state flux between the neighboring nodes with a fixed nodal distance equal to five centimeters. For a node within the soil profile, two ANN excitements are required, one for each of its neighbors. Moreover, instead of only one ANN, 25 specially trained ANNs were trained, and FIS was employed to handle instant application of the 25 ANNs. Inasmuch as the ANN estimates flux and no built-in time step is considered in its structure, any time step may be used. However, it should be kept small enough to prevent large errors, as such the sample simulation model was executed with 15 minute time steps. Although the structure of each ANN is quite small, most of the time the FIS excites more than one ANN concurrently. Overall, since the ANN-FIS-1D model contains several computational steps (caused by: small time steps, multiple ANN excitements at each time step, and FIS computations), it has higher computation cost than the ANN-1D model.

The ANN used in ANN-3D to solve the 3D problem, focuses on seven nodes at a time (one central and six neighboring), and has a four layer structure that may be presented linearly as follow:  $[I(7), H1(7), H2(15), O(1)]$ . The time step and nodal distance were both fixed values equal to 15 minutes and five centimeters respectively. The ANN was trained to receive seven initial nodal soil moisture

content values as its input vector, and to estimate the final soil moisture content for the central node. Use of soil 'moisture contents' instead of 'moisture heads' decreased the variance and contained the 'universe of possible values' within a single order of magnitude. This resulted in better ANN training. This ANN has to be excited once for each node within the flow domain at each time step. The ANN structure is smaller than those of ANN-1D (M1 and M2) and larger than that of ANN-FIS-1D. But, its computation cost is inversely related; i.e., larger than those of ANN-1D (M1 and M2) and smaller than that of ANN-FIS-1D. This is quite reasonable for the first comparison (with ANNs used in ANN-1D), because of their large time steps and the fact that those ANNs are excited only once per time step. It also makes sense for the latter comparison (with ANNs used in ANN-FIS-1D), because of the fact that it needs at least two excitements per node, plus the computation surcharge for FIS application.

Comparison of the ANN-based models reveals their pros and cons and this leads to some general conclusions. As discussed above, the ANNs used in the ANN-1D model, work with the whole soil profile. Inasmuch as the ANN is excited only once per time step, this method is fast. However, such an ANN is not mobile; i.e., it is only trained for a certain kind of profile and is not applicable to other cases. If the goal is to develop universal ANN-based VSSM redistribution simulation models, then this is a severe limitation. On the other hand, extension of this tactic to field scale 3D flow domains inflates the ANN structure, that in turn increases the computation expenses. The ANNs employed by ANN-FIS-1D model are very basic and leave many calculations for the main model which elevates the computation cost. It is mobile and with the use of FIS has been shown to be capable of solving the VSSM redistribution problem. Application of FIS has also eliminated the minor random fluctuations from the outputs of the model; such as the serration visible in ANN-3D graphs. These random oscillations are a direct results of ANN usage. Finally, the ANN trained for the ANN-3D model is mobile



and the most feasible tactic found in this study. This method provides the kernel idea. Many more efforts and improvements are needed before development of a universal ANN-based SHP simulation model is possible.

#### **ANN-BASED MODELS vs. CUSTOMARY MODELS**

This section discusses ANN-based models in contrast to customary VSSM simulation models. Customary simulation models are based on Richards' equation that in turn is an integration of 'Darcy-Buckingham' and 'Continuity' equations; therefore, it only expresses the Darcian flow. To cover for other kinds of flow, such as preferential flow and salt induced flow, customary VSSM redistribution simulation models must adopt other modules. This makes their codes cumbersome and difficult to understand. Also, for complex and/or 3D cases their computation cost increases drastically. In general, these customary models simulate the real world and attempt to explain reality to a great extent, but are not yet entirely successful. Moreover, they need detailed parameters such as hydraulic conductivity, which generally has an inherently large variance. Measurement of these parameters requires substantial time and money. Overall, high computation costs and the need of detailed input data are the most important drawback factors against customary models, specially for 3D models.

This study was aimed at exploring ANN-based alternative approaches to these customary numerical simulation practices, and to determine its feasibility in terms of veracity, computation cost, and input facilitation. ANNs learn from observed data (examples) and incorporate the real world spatio-temporal diversities directly into the model. ANN is a model-free simulation tool, which helps to minimize dependence upon pre-cast algorithms, their limitations, and their rigid parameters. It is a data-driven simulation tool capable of mimicking complex patterns and providing a direct link between real world observations and the model. Thus, renders the possibility of adoption of complexities of the real system by the model.

This study brought forth the idea that ANN-based models are competent VSSM flow simulators. If a comprehensive/universal VSSM flow database (from observed data) become available, a universal ANN-based model may be trained so as to substitute for customary numerical models. Such an ANN, is a type of model-free regression which is sensitive to individual records. Thence, it is capable of mapping all VSSM flow realities and to deal with real world diversities and data uncertainties. In fact, one of the main motives in employing ANN was to develop a model that has the ability to easily cope with the uncertainty involved in VSSM modeling.

In conclusion, the results show the possibility to model VSSM redistribution via ANN. Less computation cost, lucidity of code, simplicity of the input data requirements, and the capability to handle VSSM data uncertainty show the feasibility of the ANN-based models. However, there is a lot more to be done before total substitution of numerical models is possible with ANN-based models.

#### **REMARKS**

Although, it is theoretically admitted that multi-layer feed forward ANNs are universal function approximators, current technology has not yet provided us with a zero error ANN training tool. In fact, ANN training was found to be cumbersome and to find proper ANN structures was time consuming. Therefore, improvements in ANN training technology would be very helpful and would enhance ANN-based modeling efforts.

The size of an ANN structure is very influential with respect to computation cost, as a smaller or larger structure can directly decrease or increase the computation cost. Introduction of different soil types would increase the number of inputs and thereupon the complexity of the ANN. This means a larger ANN structure and an increase in its computation cost. Note that ANNs learn via generalization of

the regulations that relates inputs and outputs, and does not memorize the data. Break down of problem complexity is possible through application of many ANNs, each with smaller structures and specially trained for a different sub-domain of the universe of possibilities. These could then be connected via a FIS (Fuzzy Inference System) to simulate VSSM redistribution. In fact, there is a trade off here between fewer ANNs with larger structures and more ANNs with smaller structures. Overall, the computational steps should be kept minimal to increase the simulation speed.

The ANNs trained did not need the hydraulic conductivity as an input to calculate VSSM redistribution. In fact, using only one soil type gives ANN the chance to implicitly capture information, as a function of soil moisture from the soil moisture data (content or head). If more soil types are to be considered, then instead of hydraulic conductivity, some soil textural and structural data (soft/qualitative or hard/quantitative) might be used to allow the ANN to differentiate among different flow domains. This is a great advantage because elimination of such highly variable parameters saves time and money. It also allows the model to discover more information about the real system, directly from observed data.

## **CHAPTER SEVEN: CONTRIBUTION TO KNOWLEDGE**

This study investigates the usage of ANN technology, as well as FIS, as main components of a novel simulation method for Variably Saturated Soil Moisture (VSSM) redistribution modeling. Three innovative simulation models were developed and tested with simple VSSM redistribution cases in homogeneous flow domains.

The following are contributions to knowledge made:

### **1. Unsteady state modeling of VSSM redistribution phenomenon using ANN.**

Explanation: In usual modeling practices, the valueless information concealed in raw observed VSSM data are partially masked by the use of pre-defined models. ANN, as a data driven modeling tool, provides a direct connection between data and the model, without mediation of a pre-defined mathematical model. Therefore, it bestows a unique opportunity to capture whole spectra of the real world reflected within the data used.

### **2. Application of FIS for one-dimensional modeling of VSSM redistribution.**

Explanation: Real world VSSM observed data are usually associated with large variances. Therefore, temporal or spatial average representations involve high uncertainties. FIS is a well matched technique for such a situation, as it smoothes model output. Moreover, a fuzzy or linguistic format may be used for input variables via employment of FIS.

**3. Elimination of hydraulic conductivity from the list of required inputs for VSSM redistribution modeling.**

Explanation: Together, ANN and FIS, enable the model to eliminate or replace some VSSM parameters. For example, in a heterogeneous flow domain hydraulic conductivity may be replaced with some simple soil textural and structural characteristics. This will be a great help since hydraulic conductivity is highly variable through space and time, and its measurements are costly, tedious, and inherently contain large variance.

**4. Achievement of shorter execution times, especially for the 3D simulation model, in comparison to traditional numerical models.**

Explanation: Shorter execution time is essential for real time applications and/or for optimization tasks, where several executions have to be performed. Inasmuch as the novel approaches introduced in this study use ANN to estimate soil moisture redistribution they speed up the calculations. This becomes even more evident when simulating 3D cases with long simulation periods.

## CHAPTER EIGHT: RECOMMENDATIONS FOR FUTURE WORK

1. **Improvement of ANN training methods:** This is an essential prerequisite for development of a universal ANN-based VSSM redistribution model. Use of a Genetic Algorithm (GA) as an optimizer for ANN weights may decrease estimation errors; however, its time consuming nature is a disadvantage. Combination of GA and systematic optimization techniques may be useful. In any case, a zero error ANN would enhance the output of the ANN-based model.
2. **Creation of a VSSM redistribution database:** Another basic prerequisite for development of a universal ANN-based VSSM redistribution model is availability of field data. Initiation of such an effort requires establishment of a standard and inclusive format for record lines. The database project may be funded by an international agency, such as FAO or the World Bank. A very good example of what is needed (in essence) is the Unsaturated Soil Hydraulic Database (UNSODA). This project was established by the U.S. Salinity Laboratory and is claimed as "the first truly international set of retention and conductivity data". It is compiled in a relational database program published for use in the public domain. ([www.usssl.ars.usda.gov](http://www.usssl.ars.usda.gov))
3. **Use of linguistic variables:** Soil structural features with high spatio-temporal variabilities (e.g., cracks and other preferential flow paths) may be included in the database quantitatively or qualitatively. First, a standard method has to be established for any of these choices. Establishment of a linguistic/fuzzy definition is much easier than the quantitative/crisp one. This would allow inclusion of these features in the database, to eventually be used as inputs to a universal ANN-based VSSM redistribution model via FIS.

4. **Variable time step and nodal distance:** The 3D ANN-based model developed in this study used a fixed time step and nodal distance. A step forward would be to include the time step and nodal distance as ANN inputs. Faced with some computation limitations, this study used fixed values. Since, without variable time step and nodal distance, there were  $8^7 = 2097152$  possible combinations). With the use of variable time steps and nodal spaces, it is possible to speed up calculations more. That is, in the absence of sharp soil moisture gradients in space and/or time, larger values may be used for both space and time steps. Certainly huge computer resources are needed to develop an inclusive universal ANN-based VSSM redistribution model.
5. **Use of FIS:** To handle the complexity of the problem, it might be helpful to employ a FIS with multiple specially trained ANNs. This in turn decreases the size of the ANN and the computation cost. It also enables the model to receive fuzzy variables. Another advantage of using FIS is to reduce randomness in the model output, at least before a zero error ANN training method is available.
6. **Different ANNs for different events:** To break down the complexity of the problem, multiple ANNs might be trained for different events such as downward movement of a saturated front (infiltration), unsaturated downward flux, unsaturated upward flux (bare soil evaporation and/or evapotranspiration), and unsaturated horizontal flux. Each category, with certain physical similarities, limits the problem to a certain domain; therefore, the problem is lessened to describe a less general case. This leads to ease of ANN training because of less inherent generalization.