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Treatise on solute transport in porous media and its modeling for concentration-dependent permeability

Khondaker, Abu Nasser, Ph.D.

King Fahd University of Petroleum and Minerals (Saudi Arabia), 1991

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TREATISE ON
SOLUTE TRANSPORT IN POROUS MEDIA AND ITS MODELING FOR CONCENTRATION-DEPENDENT PERMEABILITY

BY

ABU NASSER KHONDAKER

A Thesis Presented to the
FACULTY OF THE COLLEGE OF GRADUATE STUDIES
KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
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In
the
name of
Allah
the Almighty
the Merciful

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DISSERTATION ABSTRACT

FULL NAME OF STUDENT : ABU NASSER KHONDAKER

TITLE OF STUDY

TREATISE ON SOLUTE TRANSPORT IN POROUS MEDIA AND ITS MODELING FOR CONCENTRATION-DEPENDENT PERMEABILITY

MAJOR FIELD : WATER RESOURCES ENGINEERING

DATE OF DEGREE : August 1991.

Solute transport in groundwater has become an active and important research area because of the increasing awareness about the living environment and the need for its protection from contamination. The amount of work, so far done in this field, is vast but scattered. Therefore, the present study has first systematically reviewed the available theoretical and experimental works since early 1950s, in particular. The review has critically analyzed the developments of research and has summarized the research trends and the associated forthcoming challenges. The review necessitates rigorous modeling of solute transport in groundwater, considering the effects of solute aggressiveness on the fundamental properties of the porous medium.

However, the modeling work is complicated and challenging because the solute transport process couples the flow of groundwater with the transport of mass in the porous medium. Because of solute aggressiveness, the hydraulic conductivity changes with concentration. Consequently, the medium becomes inhomogeneous and revises the existing concept of steady incompressible groundwater flow to an unsteady problem. The present study has modeled the groundwater solute transport incorporating these factors.

To solve the model equations, derived from the general continuity equations, permeability, porosity and concentration were correlated, and a solution algorithm, using collocation finite element technique, has been developed. The algorithm not only solves the resulting nonlinear, coupled equations under varying initial and boundary conditions but also guarantees continuous velocity field without using numerical integration.

The numerical simulation shows that the solute aggressiveness introduces additional heterogeneity in the medium, which increases the uncertainty in the estimation of hydraulic conductivity and dispersion coefficient. Increasing solute aggressiveness increases the hydraulic conductivity and the groundwater head. The existence of incompressible unsteady flow has been confirmed through numerical experiments. Therefore, the hydrodynamics of groundwater must be coupled with the associated mass transport phenomenon with special reference to modeling the effects of solute aggressiveness.

A simple experimental model was developed in the laboratory to study the dynamics of flow and transport of aggressive solutes in porous media. It was, however, not possible to study the effects of solute aggressiveness due to significant growth of microorganisms in the system.

King Fahd University of Petroleum & Minerals
Department of Civil Engineering

DOCTOR OF PHILOSOPHY

ملخص بحث

الاسم الكامل : ابو ناصر خرندا كار
عنوان البحث : دراسة نقل المذاب في الأوساط المسامية ونمذجتها للانفاذية المعتمدة على التركيز
التخصص : هندسة مصادر المياه
تاريخ الحصول على الدرجة : أغسطس ١٩٩١م .

لقد اصبح نقل المذاب في المياه الجوفية مجالاً نشطا وهاما للبحث وذلك نسبة للادراك المتزايد للبيئة المحيطة والحاجة الى حمايتها ضد التلوث ، إن حجم العمل الذي تم انجازه حتى الآن في هذا المجال كبير ولكنه مشتت . ولذلك فأن هذه الدراسة قد قامت بالمراجعات النظامية للاعمال النظرية والتطبيقية منذ عام ١٩٥٠ . وتناولت المراجعات تحليل تطورات الأبحاث وتلخيص مناهج الأبحاث والتحديات القادمة المرتبطة بذلك .

وتتطلب نمذجة المراجعة نمذجة نقل المذاب في المياه الجوفية ، بالنظر إلى تأثير ذلك في الخواص الأساسية للوسائط المسامية .

ومع ذلك ، فأن نمذجة العمل معقدة ومثيرة للتحديات لأن عملية النقل المذاب تربط بين مسألة تدفق المياه الجوفية ونقل الكتل في الوسط المسامي ويسبب النقل المذاب بتغير الداء الهايدروليكي مع التركيز ، ونتيجة لذلك يصبح الوسط غير متجانس ، وتراجع الدراسة المفهوم الحالي لدفق المياه الجوفية المنتظم وتحوله إلى غير منتظم . والدراسة الحالية تشكل نموذجاً للنقل المذاب للمياه الجوفية التي تشمل هذه العوامل . ولحل المعادلات النموذجية المستقاه من معادلات الأستمرارية العامة تم عقد مقارنة بين النفاذية والمسامية والتركيز والتوصل الى حل لوغريثمي باستعمال تقنية العناصر النهائية . ولم تساعد اللوغاريثمات في حل المعادلات غير الخطية والمقرونة فحسب ، بل ضمن أيضا مجالاً للسرعة الأستمرارية دون استعمال التكامل الرقمي .

وتبين المحاكاه الرقمية أن النقل المذاب ليضيف ايضا تنوعا في الوسط الذى يزيد من عدم مصداقية تقدير المفعول الهايدروليكي والمكافىء التشتتي . ومع ازدياد نقل المذاب تزداد الفعالية الهايدروليكية ورأس المياه الجوفية . وقد تم تأكيد وجود الدفق غير المضغوط وغير المنتظم من خلال تجارب رقمية . و لذلك يجب قرن هايدرو ديناميكية المياه الجوفية لظاهرة النقل الكتلي المرتبطة .

وتم عمل نموذج تجريبي مبسط بالمختبر لدراسة ديناميكية الدفق . نقل المذاب في الوسط المسامي . ولكن لم يكن من الممكن دراسة تأثير نقل المذاب بسبب النمو المؤثر لمايكرو اورجانيسم في النظام .

جامعة الملك فهد للبترول والمعادن
قسم الهندسة المدنية
درجة دكتوراة الفلسفة

Chapter - I

INTRODUCTION

Chapter I

INTRODUCTION

1.1 INTRODUCTION

With the increasing sense of awareness about the environment and the recognition of the need for its protection, the study of solute transport related to groundwater contamination has become the focus of numerous researchers. Specially, during the last two decades, research activities in this area have accelerated to revolutionary level.

Different investigators attacked the solute transport problem from different perspectives because it is an interdisciplinary one and the resultant achievements are so extensive and scattered that it appears to be essential to make an inventory of the completed works. A systematic inventory of the available theoretical and experimental works could make a much awaited contribution in this area. These includes :

i) brief review of the fundamental concepts of flow through porous media

ii) complete picture of the present status of the problem

iii) outlining issues that remain obscure or unaddressed by the current day investigators and

iv) suggestion of research directions and/or alternatives to advance technology for a greater understanding and a more comprehensive analyses of the solute transport phenomena.

Models, describing the solute transport in porous media , are collections of partial differential equations which contain a number of parameters, representing the aquifer properties and different processes controlling the phenomena. The success of model predictions depends on

i) the accuracy and efficiency with which the natural processes controlling the behavior of groundwater and the chemical and biological species it transports are simulated and

ii) the reliability of the estimated model parameters.

Solute transport in natural groundwater system is a coupled process , one which consists of the flow of groundwater as well as the transport of mass. Of various parameters involved, the hydraulic conductivity distribution is of major importance. Other parameters such as those related to hydrodynamic dispersion, sorption and chemical and biological transformations are important also. But the hydraulic conductivity is the most fundamental, because combined with hydraulic gradient and medium porosity, it controls the direction and speed of the moving water. These aquifer parameters are related to numerous factors including the solute characteristics and concentration.

There exists numerous models for the study of groundwater flow and solute transport problems. These are mostly developed for situations where the model parameters like hydraulic conductivity and/or hydrodynamic dispersion is considered to be independent of solute concentrations. A very few models are available for the situation of concentration-dependent permeability . In these models, the resulting nonlinear equations are developed considering the density-dependent and/or viscosity-dependent flow parameters. In other words, the existing nonlinear models are based on the concept of solute density and/or viscosity effects on flow and transport phenomena. The groundwater flow and the transport equations are coupled by the density and/or viscosity terms without changing the basic equations for the groundwater flow and solute transport. Particularly, such models assume either incompressible porous media and/or fluid system or compressible system with model parameters independent of concentration as a conventional practice. The author failed to find any flow model in the literature which considers the case of incompressible unsteady flow.

Recent studies on the effects of salinity and organic solvents on permeability indicate that an additional phenomenon, the 'solute aggressiveness' may result with a significant change of pore structures of the porous media, with or without appreciable deformation of the media or fluid. It is well understood that any activity resulting with any change in solute concentration and/or on medium porosity will definitely be associated with permeability change and ultimately a modification in the value of hydrodynamic dispersion parameter in the system. Environmental Protection Agency designated these solutes as aggressive solute or permeant (McCandles et. al.(1987)).

Literature survey also demonstrates that the solute aggressiveness is a function of a number of factors including the solute concentration (McNeal (1968), McNeal et.al. (1966,1968), Pupisky & Shainberg (1979), Abu-Sharar et.al.(1987), Brown & Thomas (1984,1987), McCandless et.al.(1987)). Depending on the nature of the media as well as the solute, either reduction or increase in the values of the flow and transport parameters are reported. This modification may be irreversible (Goldenberg et.al. (1983) or may show a hysteresis nature (Mehnert & Jennings (1985)). In any case, the resulting effect is the change of the media from homogeneous to heterogeneous or increase in heterogeneity in case of heterogeneous media.

One of the most important problem that is unresolved to date is the assessment of any reliable correlation between the field and the laboratory values of the flow and the transport parameters.

According to most investigators, the principal cause of the existing discrepancy between the field and the laboratory values of model parameters is the heterogeneity of the medium (Taylor et.al (1987), Poley (1988)). In case of aggressive solutes, the change of parameters with solution concentration introduces additional heterogeneity, even in the case of a medium which may be homogeneous by nature. In such a situation, the non-existing relationship between the field and the laboratory values of such parameters might get worse. This problem can only be treated if a careful study of solute aggressiveness is performed and analyzed properly. A successful study in this direction may explain to some extent the cause of the failure to asses any definite relationship between the field and the laboratory values of flow and transport components.

According to Hassanizadeh et.al. (1988), the existing models employ assumptions and approximations which are not admissible at high concentrations. Solute aggressiveness is a function of concentration and the limiting case may be at high concentrations. Theoretical studies indicate that for high-concentration, as well as in the case of aggressive solutes, one might need to modify the basic equations of flow and transport.

The purpose of this research is to illustrate and stress the need for more careful examination of ideas, equations and methodologies applied for modeling of aggressive solute transport problems.

The most important aspects of the mathematical model i.e. the basic equations, will be reviewed carefully. A modified formulation of the equations will be proposed . A suitable solution algorithm will be developed to solve the resulting system of nonlinear equations using advanced numerical technique. The effects of the proposed modifications will be illustrated by means of numerical experiments.

An attempt to study the dynamics of flow and transport of aggressive solutes in the laboratory would be considered.

1.2 BRIEF LITERATURE REVIEW

The study of groundwater flow and the contaminant transport requires the knowledge of many of the basic principles of geology, physics, chemistry and mathematics. From the theory and the solute transport point of view, there exists a close kinship between groundwater hydrology, soil mechanics, rock mechanics, physical chemistry, mathematics and petroleum engineering.

Different attempts have been taken by the respective disciplines according to their needs, but the physical processes they apply are the same in most of the cases. Although such studies related to groundwater contamination are not very old as an applied science problem, almost similar studies originated long ago in chemistry, soil science and other scientific disciplines.

Solute transport in natural groundwater systems is a coupled process which consists of the flow of groundwater as well as the transport of mass. According to some investigators (Konikow and Grove (1977)), the solute transport problems should be treated simultaneously with the groundwater flow because of their close kinship.

With the increasing sense of environmental protection , the solute transport problem, particularly in groundwater contamination gradually received increasing attention of the various researchers which resulted in an extensive volume of work to date. It appears to be advantageous to discuss them under the different categories, namely:

a) Theory and Development of Solute Transport Phenomena

b) Studies on Aquifer Properties

c) Modeling of Solute Transport
d) Parameter Identification and Tracers
e) Macrodispersion and Stochastic Approaches
f) Transport in Fractured Media
g) Analysis of Field Problems
h) Aquifer Reclamation and Management Aspects

As the proposed research also includes an inventory of the completed works, a few of the works most relevant to this proposed research are mentioned below (a more detailed review will be presented in the following sections of this study). A broad list of related works are also available in Khondaker (1989) and Khondaker et.al. (1990).

The birth of groundwater hydrology as a quantitative science can be traced to the year 1856 when a French hydraulic engineer, Henry Darcy published his report describing a laboratory experiment that he carried out to analyze the flow of water through sands. The results of his experiment can be generalized into the empirical law that now bears his name.

Darcy's law , being an empirical one, resting only on experimental evidence, it was necessary to derive Darcy's law from more fundamental physical laws and the most successful approaches attempt to apply the Navier-Stokes equations, which are widely known in the study of fluid mechanics, to the flow of water through the pore channels of idealized conceptual models of porous media. The earliest attempt to verify Darcy's law by analytical means were carried out by Hubbert(1956) and Irmay (1958).

In the related literature, the earliest observation of the dispersion phenomena is reported by Slichter (1905) who used an electrolyte as tracer in studying the movement of groundwater. Remarkable studies on related processes in groundwater flow and contamination transport appear to begin from 1950 and followed by numerous studies in the fields of soil science, chemistry ,hydrogeology and petroleum engineering.

Among the potential contributors in the development of theory of groundwater flow and solute transport phenomena, the names of Saffman (1959,1960), Scheidegger (1961), Deans (1963), Bachmat & Bear (1964,1972), Ogata (1970)) appear to be in the forefront. Bear (1961) also worked on experimental studies of dispersion phenomena in porous media. Also Bear (1972,1979) presented very systematic development of groundwater flow and solute transport phenomena in porous media. Other investigators (Pinder et.al.(1973), Pinder (1984), Whitaker (1973), Gray (1975), Konikow & Bredehoeft (1978), Hassanizadeh (1986,1986a), Konikow & Mercer (1988) etc.) also presented formulations that are basically similar to Bear (1972,1979).

Among a number of investigators who are working on the experimental determination of model parameters, Van Genuchten's (1981,1984,1984a) contribution appears to be acknowledged first.

McNeal and Coleman (1966), McNeal (1968), McNeal et.al. (1966,1968) presented their experimental findings on the effects of solute composition and characteristics on hydraulic conductivity. Abu-Sharar et.al. (1987) also presented a study on the reduction of hydraulic conductivity in relation to clay dispersion and disaggregation. Brown & Thomas (1987) explained a mechanism by which the organic liquids increases the hydraulic conductivity of compacted clay materials. Chen et.al.(1987) studied the effects of organic compounds on swelling and flocculation of Upton Montmorillonite. These studies were carried out from the field of soil science.

The study on the effects of solute aggressiveness on the properties of porous media related to solute transport was originated from the work of Anderson (1982). When compared to water, clay liners exhibited an increase of permeability by a factor of one million. Brown and Thomas (1984) presented a study showing the increase in hydraulic conductivity of clays to petroleum products and organic solvents. After that Environmental Protection Agency initiated and supported a number of research projects in this direction (Brown and Anderson (1983), McCandless,et.al.(1987),Brown (1988),Miller (1988)). All of the aforementioned studies clearly indicates the significance of solute aggressiveness and the need to incorporate this phenomena in future solute transport studies. But the extensive literature survey amply demonstrates the absence of such a model. In addition, a very few models are available for natural coupled system of groundwater flow and transport.

1.3 PRESENT STATUS OF THE PROBLEM

The capability to predict the behavior of chemical contaminants in the flowing groundwater is of vital importance. The reasons are:

i) the need for reliable assessment of hazards or risks arising from groundwater contamination problems, and
ii) design of efficient and effective techniques to mitigate them.

The widespread use of chemical products, coupled with the disposal of large volume of waste-materials, poses the potential for widely distributed groundwater contamination. For example, hazardous chemicals eg. pesticides, herbicides and solvents are used ubiquitously in everyday life. These and a host of other chemicals are in widespread use in urban, industrial and agricultural settings.

Whether intentionally disposed of, accidentally spilled, or applied to the ground for agricultural reasons, some of these chemicals can eventually reach the groundwater and contaminate it. Because of the volume of toxic wastes and of their stability in the subsurface environment, such contaminants can pose a serious threat to public health. Groundwater acts as a transporting agent for dissolved chemicals including contaminants. The major geophysical inputs to the problem of waste disposal and groundwater contamination deal with the chemistry and rates and direction of contaminant transport.

The most challenging problems associated with groundwater contamination are:

1. to prevent the introduction of contaminants in an aquifer

2. to predict their fate and movement if they are introduced
3. to remove them, thereby, protecting the biosphere effectively.

These problems are the results of our yesterday's mistakes, today's necessity and tomorrow's protection.

In order to rectify these problems, future research is needed for the followings :

i) understanding of physical, chemical and biological processes controlling the fate and movement of contaminants in the subsurface environment

ii) the mathematical representation in the transport models to predict the contaminant movement

iii) determination of different important model parameters in the field and the laboratory using alternative methods

iv) development of transport models to predict the movement of contaminants as they are introduced

v) development of management models to control and/or prevent the introduction of contaminants in the aquifer and to find the methodology for safe disposal of hazardous wastes.

vi) removal of contaminants to some extent possible to protect the biosphere effectively.

Extensive research works have been reported in literature in different directions and from different disciplines of science and technology. In spite of all these efforts, continuous research is still needed to overcome the present limitations of the available models . Because, it must be admitted at the outset that simulation models are not truly predictive tools in a classic scientific sense. It appears that the use of mathematical models to simulate the behavior of any complex natural system lies somewhere between science and art. Therefore, modeling of such natural systems is a never-ending activity in that improvements are continually being made as more understanding and information become available.

The extensive literatures available appears to be considerably scattered because the problem is an interdisciplinary one. Therefore, there exists a need for a systematic inventory of available theoretical and experimental works which would be able to make a much awaited contribution in this area (van Genuchten (1988)).

In spite of all these efforts, there exists a need for continuous research in a number of directions to reduce the present limitations and uncertainties associated with predicting the fate and the behavior of contaminants in the subsurface (Khondaker et.al. (1990)).

Modeling of aggressive solutes appears to be among the most potential directions of research to be pursued. This is because, the effect of solute aggressiveness on the two aquifer properties is of vital importance. Furthermore, since the hydraulic conductivity depends on the void ratio and the fluid viscosity, any changes in these two properties will change the hydraulic conductivity and in turn will affect transport.

The general solute transport equation relates concentration changes to hydrodynamic dispersion, convective transport, fluid sources and sinks, and chemical reactions. Because both dispersion and convection transport depend on the velocity of the groundwater flow, the solute transport equation must be solved in conjunction with the groundwater flow equation (Konikow and Grove (1977), Konikow & Bredehoeft (1978)). A few work have been reported in this coupled process (Huyakorn & Taylor (1976), Anand et.al.(1980), Anand & Pandit (1982), Mehnert & Jennings (1985)). Most of these models employ assumptions and approximations which are not admissible at high-concentration or in aggressive solute transport problems. Hassanizadeh & Leijnse (1988)) presented a model of brine transport in porous media . They considered the effects of high concentration on permeability due to solution viscosity keeping the porosity constant. The studies on the effect of solute aggressiveness on porous media indicates that the aggressive solutes change hydraulic conductivity by several orders of magnitude, significantly different from that caused by density and viscosity variations. Such a change appears to be related to the change in intrinsic permeability and thereby the porosity.

Furthermore, a very few models are reported in the literature which solves the natural groundwater system, which is in fact a coupled system of flow and transport. Almost all of these models used finite difference and the Galerkin finite element techniques to solve the governing equations. It is obvious that the simultaneous solution of the equations governing the coupled natural system requires more reliable solution technique since the one equation utilizes the results of the other one throughout the solution process. Finite difference method and/or Galerkin finite element method with linear interpolation function does not guarantee a continuous head gradient distribution to be used in the evaluation of the velocity field needed to solve the transport equation. Use of advanced numerical techniques appears to be a successful attempt to overcome this difficulty.

Therefore, there exists a need for the development of a model to predict the transport of aggressive solutes by solving the diffusion-convection equation coupled with the groundwater flow equation including various processes involved and considering the potential effects of solute aggressiveness on aquifer properties of vital importance.

1.4 RESEARCH OBJECTIVES:

This research is intended to achieve the following objectives :

1. A systematic inventory of completed works
2. Modification of the basic equations of groundwater flow and solute transport to incorporate the new concepts of solute /permeant aggressiveness and incompressible unsteady flow condition.
3. Development of a general purpose numerical model which will be capable to deal with the nonlinear problem of solute transport in groundwater using the diffusion-convection equation coupled with the groundwater flow equations for
    a) Concentration-dependent permeability
    b) Incompressible unsteady groundwater flow of aggressive solutes.
    c) Compressible unsteady groundwater flow of aggressive solutes
4. Comparison of the developed model with the conventional results to establish the viability of the new concepts mentioned in item-(2) above.
5. A parametric study to illustrate the effects of solute aggressiveness on flow dynamics and solute dispersion pattern of an aquifer by means of numerical experiments.

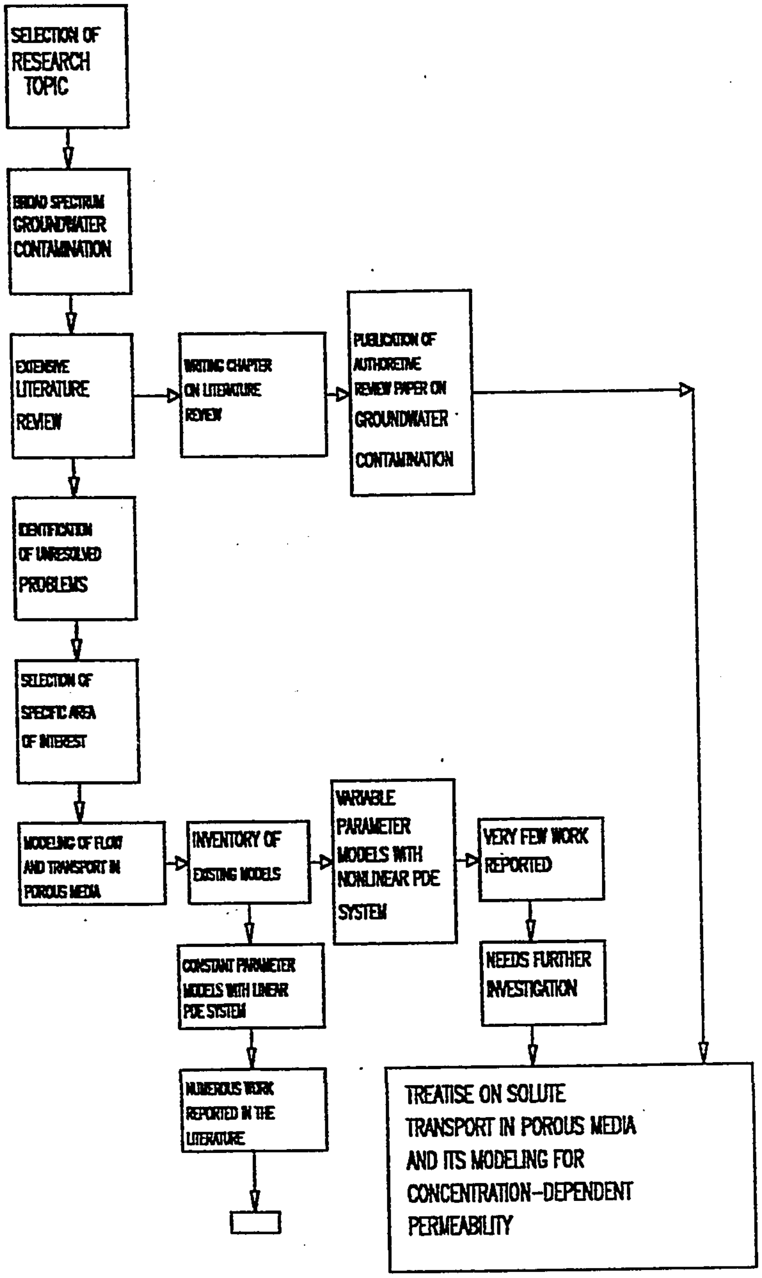

Figure 1.1 : Summary of Research Proposal

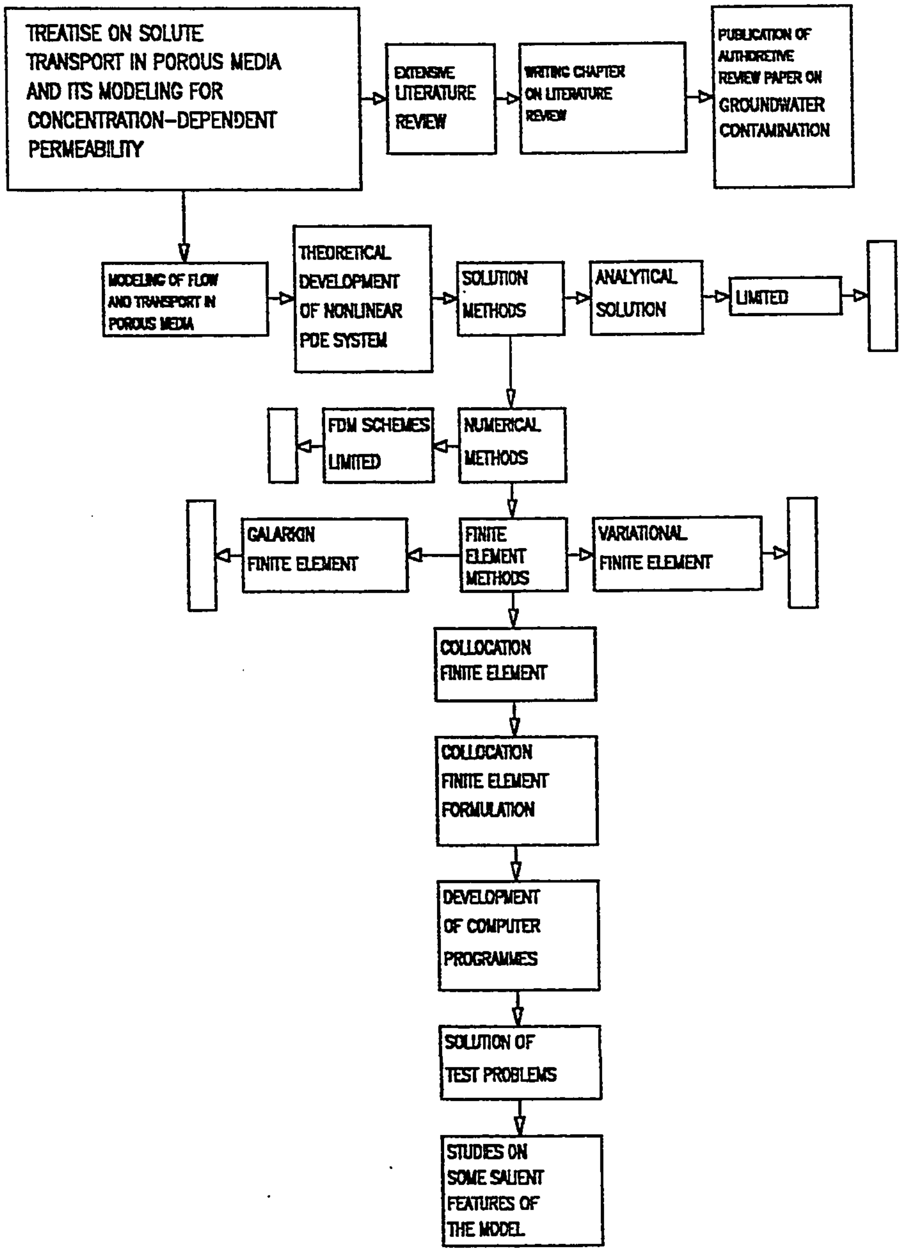

Figure 1.2 : Summary of Research Outlines

Chapter II

LITERATURE SURVEY
AND THE STATE-OF-THE-ART OF THE PROBLEM

Chapter II

LITERATURE SURVEY AND THE STATE-OF-THE-ART OF THE PROBLEM

2.1 INTRODUCTION

The capability to predict the behavior of chemical contaminants in flowing groundwater is of vital importance for a) the reliable assessment of hazards or risks arising from groundwater contamination problems, and b) the design of efficient and effective techniques to mitigate them.

Reliable and quantitative prediction of contaminant movement can be made only if we understand the processes controlling the transport of contaminants. These include a) advection b) hydrodynamic dispersion and c) physical, chemical and biological reactions that affect their soluble concentrations in groundwater

The widespread use of chemical products, coupled with the disposal of large volume of waste-materials , pose the potential danger of groundwater contamination. New instances of groundwater contamination are continually recognized. Hazardous chemicals (e.g. pesticides, herbicides, and solvents) are used ubiquitously in everyday life. These, and a host of other chemicals, are in widespread use in urban, industrial, and agricultural settings.

Whether intentionally disposed of , accidentally spilled , or applied to the ground for agricultural reasons, some of these chemicals may eventually reach the groundwater and contaminate it, causing a serious threat to public health.

Groundwater is the subsurface transporting agent for dissolved chemicals including contaminants. Material dissolved from wastes may be transported from burial or disposal sites by groundwater flow, affecting the quality of subsurface water.

In addition, natural discharges of an aquifer, such as springs and seeps, can return contaminants to the surface. Because of the relatively slow rates of groundwater movement and the natural flushing of aquifers, those contaminants could remain for a long time.

The major geophysical inputs to the problem of waste disposal and groundwater contamination deal with the chemistry, rates and direction of contaminant transport. The most challenging problems associated with groundwater contamination are :

1. to prevent the introduction of contaminants in an aquifer;
2. to predict their movement if they are introduced; and
3. to remove them, to some extent in order to protect the biosphere effectively.

These problems are the results of yesterday's mistakes, today's necessities and tomorrow's protection.

If groundwater is to be utilized safely and effectively, both increased scientific knowledge and improved engineering techniques must be brought to bear on the problem of groundwater contamination. The development of appropriate methods for managing and disposing of wastes are necessary for rectification of past mistakes and for future protection as well.

The scientific problem is one of understanding the physical, chemical, and biological system sufficiently well to be able to predict the movement and fate of contaminants . This challenge is not met easily, but with concentrated effort, it should be possible to isolate some toxic substances in the groundwater under certain conditions in a way that will pose no hazards to the environment.

Subsurface flow and contaminant transport continue to be studied in some branches of science including groundwater hydrology, petroleum engineering, soil science, and to some extent chemical engineering.

While the applications of scientific knowledge in these disciplines often differ, the physical processes that apply are the same in most of the cases. These disciplines complement one another, and to a large extent, technology has been shared by them.

With the increasing sense of environmental protection, the study of groundwater contamination has become the focus of numerous researchers. A revolution in investigation schemes has appeared in related literature. Investigators have attacked the problem from different angles and the resultant achievements are so scattered that it is essential to inventory such investigations (Figure 2.1 and Table 1). This is necessary to provide a complete picture about the present status of the problem and identify the directions of research needs in the future.

A qualitative presentation of reported works is shown in Figure-2.1. This figure is based on a collection of more than a thousand articles (Khondaker,1989).

The presentation of this study is divided into three different sections:

1. General
2. Research Directions
3. Identification of unresolved Problems

The statistics of articles examined under the above sections are shown in Table-1.

Table-1 : The number of publications examined during the literature survey

Section	--> 1959	1960-1969	1970-1979	1980-1988	Total
General	--	2	27	52	81
Theory and Development of Solute Transport Phenomena	15	30	70	282	397
Modeling of Solute Transport	3	20	154	207	284
Studies on Model Parameters	2	20	33	79	136
Total	**20**	**72**	**286**	**623**	**1001**

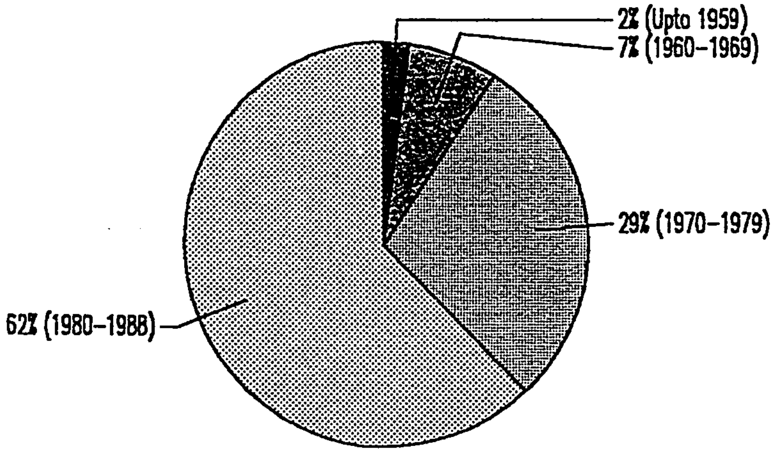

Figure-2.1 : Publication periods of over 1000 articles related to Groundwater Contamination studies (Khondaker (1989)).

2.1.1. General

Groundwater contamination studies generally include:

i) the scientific understanding of physical, chemical, and biological processes controlling the fate and movement of contaminants in the subsurface environment;
ii) the mathematical representation in the transport models to predict the contaminant movement;
iii) the determination of different model parameters in the field and the laboratory using different methods;
iv) the development of transport models to predict contaminant movement if they are introduced;
v) the development of management models to control and/or prevent the introduction of contaminants in the aquifer and to determine the methodology for the safe disposal of hazardous wastes, and
vi) the development of methodology for the removal of contaminants to the extent necessary to effectively protect the biosphere.

Therefore , the study of groundwater flow and the contaminant transport requires knowledge of many of the basic principles of geology, physics, chemistry, and mathematics. There is a close kinship between groundwater hydrology, soil physics, soil mechanics, rock mechanics, and petroleum engineering.

The earliest observation of the dispersion phenomena was reported by

Slichter (1905) who used an electrolyte as a tracer to study the movement of groundwater. Remarkable studies on related processes in groundwater flow and contamination transport started in 1950 and gradually received the increasing attention of researchers. This review includes articles roughly from 1950 onwards.

2.2 RESEARCH DIRECTIONS

During the past two decades, a great deal of effort has been directed toward the understanding and quantification of physical and chemical processes which affect the subsurface transport of contaminants. Once primarily the realm of hydrologists, the field of contaminant transport study has mushroomed in scope to include soil scientists, chemists, biologists, petroleum engineers, mathematicians, and statisticians. The outcome of these studies from different disciplines complement one another. These studies can be broadly classified into the following categories:

a) theory and development of solute-transport phenomena,
b) modeling of solute transport, and
c) studies on model parameters

The above classification is somewhat arbitrary since some of the works span more than one category. However, this categorization permits a more systematic presentation of the large number of relevant papers.

2.2.1 Theory and Development of Solute-Transport Phenomena

From the theory and the solute transport phenomena point of view, there exists a close kinship between groundwater hydrology, soil mechanics, rock mechanics , physical chemistry, mathematics, and petroleum reservoir engineering. The birth of groundwater hydrology as a quantitative science can be traced to 1856 when a French hydraulic engineer, Henry Darcy, published his report describing a laboratory experiment that he carried out to analyze the flow of water through sands. The results of his experiment can be generalized into the impirical law that now bears his name. Darcy's law , being an empirical one, rests only on experimental evidence, therefore, it was necessary to derive Darcy's law from a more fundamental physical law. The earliest attempt to apply Navier-Stokes equations, which are widely known in the study of fluid mechanics, was made by Hubbert (1956) and Irmay (1958).

Among the potential contributors in the development of theory of groundwater flow and the solute transport phenomena, the names of Saffman (1959, 1960), Scheidegger (1961), Deans (1963), Bachmat and Bear (1964, 1972), and Ogata (1970) appear in the forefront. Bear (1961) also worked on experimental studies of dispersion phenomena in porous media. Bear (1972, 1979) presented very systematic development of groundwater equations and solute transport phenomena in porous media. Other investigators (Bredehoeft and Pinder, 1973; Pinder, 1984; Whitaker, 1973; Gray, 1975; Konikow and Grove, 1977; Konikow and Bredehoeft, 1978; Hassanizadeh, 1986, 1986a; Dagan, 1987; Konikow and Mercer, 1988) also presented formulations that are basically similar to Bear (1972, 1979).

A proper understanding of the simultaneous movement of water and solutes in porous media is essential for i) improved efficiency of soil-applied agrochemicals, ii) prevention/prediction of groundwater contamination, iii) safe waste disposal site management, and iv) wastewater renovation.

In order to satisfy the increasing demand of the above necessity, identification of the following processes must be made.

a) advection (convection)
b) diffusion
c) dispersion
d) sorption and retardation/decay
e) chemical reactions
f) biological reactions
g) ion exchange

The conceptual definition of all these processes was presented by many authors in different standard texts (Fried and Combarnous, 1971; Bear, 1972; Freeze and Cherry, 1979). Comprehensive reviews of these processes in the context of groundwater contamination studies was presented by a number of investigators (Nielson et al., 1981; Roberts et al., 1982; Davidson et al., 1983; Anderson, 1984; Abriola, 1987).

2.2.2 Modeling of Solute Transport

A model designed to simulate a physical system generally begins with a conceptual study based on the understanding of the processes (cause-effect) which accounts for the behavior of the physical system. From this conceptual model, a set of mathematical equations can be developed that are subject to initial and boundary conditions, and which represent the operation of the physical system. Finally, the equations are solved and the results evaluated.

When all equation subsets are defined, two approaches are available to solve the mathematical model, namely the analytical and the numerical methods. Analytical methods are applicable to limited cases of simplified problems. Investigators have established, through laboratory and field experiments ,that prediction of subsurface transport is much more complex than heretofore imagined. These complications and the persistence of contaminants in groundwater has led to increasing specialization within the field of transport modeling. To overcome the limitations of analytical approaches, two popular numerical techniques have emerged; the finite difference and the finite element methods.

Several hundred models are available to investigate groundwater contamination. Indeed, no individual can hope to have an in-depth understanding of all phenomena. Hence numerous models are available as a result of different concepts and/or combinations of processes involved.

Bachmat et al.(1980) conducted a survey of numerical models mainly related to groundwater management. His report contained a list of 138 flow models and 39 mass transport models in 14 countries. Naymik (1987) presented a systematic review of 44 technically advanced articles on mathematical modeling of solute transport in the subsurface system. His review covers the period 1980-1985 only. Another comprehensive review paper on modeling of solute transport in groundwater was presented by Abriola (1987). She reviewed models reported up to 1986.

In order to compress the volume of this paper, articles published in 1987 and thereafter were considered too highly focused to be included. An inventory of different models are presented in Appendix-A1 (Grove and Stollenwerk, 1987; Bachmat et al., 1980).

Angelakis et al.(1987) described simultaneous transformation and transport of two solutes with different dispersion coefficients by two one-dimensional partial differential equations. They used the linear equilibrium adsorption-desorption relationship for both solutes and irreversible microbial first-order kinetics as an overall transformational mechanism. Analytical solutions were obtained using Laplace transformation for zero initial conditions, pulse input conditions, and semi-infinite media. Sensitivity of the concentration profiles of both solutes to their respective dispersion coefficients were also presented. This model offers an opportunity to study the transport and transformation mechanisms of two solutes without the necessity of assuming that the dispersion coefficients are equal, as is the case for most existing models. Bouwer and Cobb (1987) presented a model to simulate biological processes in the subsurface system incorporating external mass transport effects.

Chen (1987) derived an analytical solution for the radial dispersion case. Dagan (1987,1988) presented a comprehensive review and evaluation of solute transport by groundwater. Galya (1987) derived a model to simulate three dimensional contaminant transport from a horizontal plane source. He used Green's function and incorporated retardation and decay. His model is also able to simulate varying source emission rates. Grenny et al. (1987) developed a mathematical model for evaluating the fate of hazardous substances in an unsaturated soil zone. The processes incorporated include volatilization, degradation, adsorption/desorption, advection, and dispersion in four phases. Model predictions were compared with laboratory soil column experiments. Heinrich and Yu (1987) claimed numerical diffusion and dispersion free , second-order time and third-order space accuracy, in their model using the Petrov-Galerkin finite element method. They solved simple one-dimensional convection-diffusion equation. Schulin et al.(1987) worked on the transport of two conservative tracers , bromide and chloride, in a stony field soil under natural conditions. They analyzed the data using classical convection-dispersion equation and a regional stochastic model that assumes a logarithmic distribution of pore water velocity and dispersion coefficients across the field.

Andersen et al.(1988) presented the results of numerical modeling of salt-water intrusion at Hallandale, Florida. They used a series of three numerical models : the cross-sectional model, the regional model, and the well field model.

Hassanizadeh and Leijnse (1988) worked on modeling of brine transport in porous media. They discussed certain important physical and mathematical differences between low and high concentration situations. They solved a set of two nonlinear coupled partial differential equations obtained from a modified formulation of Darcy's and Fick's laws by means of iterative methods. Lassey (1988) derived an analytical solution to the advection-dispersion equation for one-dimensional solute or tracer transport including sorption and first-order loss. Miller and Weber(1988) and Weber and Miller (1988) described laboratory investigations and mathematical modeling of the sorption of hydrophobic solutes by aquifer materials. They obtained accurate representations of the sorption process with either a dual resistance diffusion model or an equilibrium /first-order sorption rate model. Russo (1988,1988a) worked on numerical analyses of the nonsteady transport of interacting solutes through undisturbed soils , both homogeneous and layered systems. His work was based on the assumptions of single-phase, one-dimensional vertical transport of a solution under isothermal and isobaric conditions in an infinitesimal , incompressible unsaturated-saturated element of soil system. Srinivasan and Mercer (1988) worked on simulation of biodegradation and sorption processes in groundwater. They presented a one-dimensional finite difference model for simulation in a saturated porous media. They formulated a nonlinear model that is capable of accommodating a variety of boundary conditions and process theories. Symons et al.(1988) presented their laboratory batch reactor generated quantitative information about the fate of polynuclear aromatic hydrocarbon compounds in soil systems. They used Grenny's (1987) model for the determination of the first-order degradation rates and equilibrium partitioning coefficients from the laboratory data. Widdoson et al.(1988) developed a system of nine coupled nonlinear equations to simulate organic carbon biodegradation by facultative bacteria in saturated porous media. They used a solution technique which is highly resistant to numerical dispersion and oscillation when applied to advection-dispersion equation even for a large Peclet number. They presented results from hypothetical experiments.

It can be concluded from the above review that recent investigators are more interested in additional phenomena involved in the subsurface solute transport process. Most recent works focused on unsaturated media and biological processes. The stochastic modeling approach has also received considerable attention of researchers.

Problems associated with modeling of solute-transport phenomena

Models are collections of partial differential equations that contain a number of parameters which represent an aquifer's physical properties. These properties must be measured in the field so that the simulated results can be verified to represent the real situation as closely as possible.

Of the various parameters involved, the hydraulic conductivity distribution is of major importance (Molz et al., 1987). Other parameters relating to sorption, hydrodynamic dispersion, and chemical and biological transformations are important as well, but hydraulic conductivity is more fundamental because, when combined with the hydraulic gradient and medium porosity, it relates to the fundamental mechanism of flow.

Variations in hydraulic conductivity with depth results in significant variations in groundwater flow and transport velocities. It is the resulting velocity variations that give rise to apparent scale-dependency of dispersion. Theoretical and experimental studies indicate that the variation of horizontal hydraulic conductivity with respect to vertical position is the key aquifer property relating to the spreading of contaminants (Molz et al., 1987).

Therefore, the development of any accurate and efficient solute transport model requires:

i) an understanding of the physical,chemical and biological system, and
ii) the conceptualization and measurement of important aquifer properties such as hydraulic conductivity distribution and the relationship of such measurements to dispersion (spreading) of contaminants in aquifers.

The major problem in the modeling of solute transport is the uncertainty associated with the values of aquifer properties to be used in model calibration and simulation. In most cases, these values are determined in the laboratory and there exists no well-defined correlation between values in the laboratory and the field.

Besides, the solute transport being a natural phenomena involving numerous environment-dependent physical, chemical, and biological activities, it is impossible to simulate all properties in a model. Therefore, the validity of the assumption made to reduce the complexities of the phenomena is of paramount importance in modeling solute transport .

2.2.3 Limitations of the existing models:

Although numerous researchers are engaged in developing solution algorithms, continuous research is still needed to overcome the present limitations of available algorithms . These limitations include:

1. Most available models are developed using laboratory conditions which cannot reliably predict the fate and movement of contaminants in the field.

2. In most of the cases, the processes include advection,dispersion , adsorption, and retardation/decay (Beljin, 1986). Very few models are available which consider the process of biodegradation.

3. Nearly all existing models consider concentration as an independent parameter from permeability and dispersion . Studies on the effect of organic solvents on permeability suggest the necessity of modeling solute transport in groundwater for concentration-dependent permeability and dispersion.

4. Available models incorporating the biological processes do not consider the effect of biological processes on aquifer properties like permeability and dispersion. It is clearly understood that biological activities resulting in any change in the chemical contaminant and/or on medium porosity, will definitely be associated with a permeability change and, ultimately a modification in the dispersion coefficient. Presently, there exists a need for such a model which will incorporate all of these modifications related to aquifer properties.

5. Most existing models, analytical or numerical, are limited to certain Peclet number. At high Peclet number, the transport equation behaves like wave-type hyperbolic equation and the existing models experience oscillations.

2.2.4 Studies on Model Parameters

The accuracy of model predictions depends on the reliability of the estimated model parameters. Unfortunately, these parameters are not directly measurable from a physical point of view and an averaging over some scale is always necessary. Besides, there exists no well defined relationship between field and laboratory values of contaminant flow parameters (Taylor et al., 1987). Hence various inverse methods have been developed for parameter identification. In these methods, the parameters used to derive the governing equation(s) are optimally estimated from observations made on dependent variables along with appropriate initial and boundary conditions.

Various techniques have been developed for parameter estimation by different methods including the solution of the inverse problem in groundwater. Carrera and Neuman (1986a,1986b,1986c) presented algorithms for the estimation of aquifer parameters under transient and steady state conditions using the maximum likelihood method. They applied their algorithms to synthetic and field data. Chin (1986) also worked on the estimation of dispersion coefficient in porous media. Wagner et al. (1986) reported a statistical methodology for estimating transport parameters. Jabson (1987) presented a method of estimating dispersion and first-order rate coefficients using numerical routing. Kool et al. (1987) reviewed parameter estimation procedures for unsaturated flow and transport models. Loaiaga and Marino (1987) used a system of simultaneous equations as a consistent estimator of unknown parameters in confined aquifers. Mehran et al.(1987) worked on distribution coefficient of trichloroethyline in a salt water system. A detail of inverse techniques is available in Yeh (1986) and Yeh and Wang (1987).

The aquifer properties of vital importance in the studies of groundwater contamination are permeability, hydrodynamic dispersion, adsorption, reaction rate, and the distribution coefficients. Numerous studies are reported in the literature on these parameters from the fields of soil science, chemistry, hydrogeology, and petroleum engineering. A brief review of selected works covering the determination of the model parameters is presented below:

Among a number of investigators who are working on the experimental determination of model parameters, van Genuchten's (1981,1984,1984a) contribution appears to be acknowledged first. Sillman et al.(1987) investigated the longitudinal dispersion in anisotropic porous media in the laboratory.

Bachmat et al.(1988) developed a theoretical technique for the evaluation of aquifer parameters using a single-well tracer test. Mukhapadhyay (1988) presented an automated computation procedure for parameters for leaky aquifers. Rowe et al.(1988) worked on the laboratory determination of diffusion and dispersion coefficients of contaminants using undisturbed clay soils. Very few works have reported on the correlation between field and laboratory values of different model parameters. Taylor et al.(1987) failed to establish any reliable correlation between field and laboratory values of such parameters.

Lambert (1967) presented the functional relationship between sorption in soil and chemical structure. Briggs (1969) worked on sorption of herbicides by soil. Hance (1969) presented an empirical relationship between chemical structure and the sorption of some herbicides. Bailey and White (1970) reported their studies on the influence of different factors on adsorption, desorption and movement of pesticides in soil. Briggs (1970) presented a relationship between soil sorption of organic chemicals and their octanol/water partition coefficients. Chiou et al. (1977) worked on partition coefficient and bioaccumulation of organic chemicals. Kirkhoff et al. (1979) presented adsorption isotherms for a series of hydrophobic compounds. Kirkhoff (1981) worked on semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments. A number of studies on adsorption were also reported (Gupta, 1974, Lin (1977.1977a), Travis,1978, Fu et al., 1983, Gupta and Bhattacharya, 1983, Rao and Jessup, 1983)). Recent studies on adsorption were reported by Curtis et al. (1986), Elabd et al. (1986), Kinniburgh (1986), Mackay et al.,(1986), Borden and Bedient (1987) and Weber and Miller (1988).

A number of investigators have considered the effect of solute concentration and composition on aquifer properties. McNeal and Coleman (1966), McNeal (1968) and McNeal et al.(1966,1968) presented their experimental findings on the effects of solute composition and characteristics on hydraulic conducivity. Abu-Sharar et al.(1987) presented a study on the reduction of hydraulic conductivity in relation to clay dispersion and disaggregation. Brown and Thomas (1987) explained a mechanism by which organic liquids increase the hydraulic conductivity of compacted clay materials. Chen et al.(1987) studied the effects of organic compounds on the swelling and flocculation of Upton Montmorillonite. These studies were carried out in the field of soil science.

The study of the effects of solute aggressiveness (McCandless et al.,1987) on the properties of porous media related to solute transport originated from the work of Anderson (1982). When compared to water, clay liners exhibited an increase of permeability by a factor of one million. Brown and Thomas (1984) presented a study showing the increase in hydraulic conductivity of clays to petroleum products and organic solvents. Later, the U.S. Environmental Protection Agency initiated and supported a number of research projects in this direction (Brown and Anderson, 1983; McCandless et al., 1987; Brown, 1988; Miller , 1988). These studies clearly indicate the significance of solute aggressiveness and the need to incorporate this phenomena in future solute transport studies.

2.3 IDENTIFICATION OF UNRESOLVED PROBLEMS

Groundwater, which is ubiquitous in the crust of the Earth, serves not only as a widely distributed source of water but as a host and transporting agent for contaminants. Although research continues and numerous works have been reported in the related literature, scientific understanding of the chemistry and transport of contaminants in groundwater is inadequate to reliably predict the fate and behavior of the contaminants.

Since the problem is an interdisciplinary one, the available extensive literature is quite scattered. There exists a need for a systematic inventory of available theoretical and experimental works (van Genuchten, 1988). Furthermore, research is needed on the effects of chemical reactions on transport and dispersion of contaminants by groundwater and the quantification of flow in fracture media.

There exists a number of important areas which need further research to predict the fate and the behavior of contaminants in the subsurface system. Some of them are;

1. Most available models are derived to simulate idealized (laboratory-scale) conditions and often do not apply to undisturbed field systems because of macropore flows and/or large scale spatial variability effects. Additional work to derive field-scale models is essential if we are to address the long term problem of soil and groundwater pollution (van Genuchten, 1988).

2. This literature survey amply demonstrates that there exists a need to derive a correlation between field and laboratory values of the various parameters used as input to solute transport models, particularly those for hydrodynamic dispersion and hydraulic conducivity. Few works have been done in this area

and no reliable correlation is reported. A successful study in this area would result in a reliable correlation between field and laboratory values of such parameters and would eliminate the need for extensive field experiments.

3. Continued investigation of the geochemistry of contaminant reactions in both saturated and unsaturated subsurface environment is necessary. Certain organic contaminants appear to be particularly persistent in groundwater and are hazardous at low concentrations. Many organic reactions are biologically controlled. At present, the role of microorganisms in solute transport in the subsurface system is poorly understood. Only a limited number of situations and organic compounds have been investigated (Fries and Marrow,1984, Hankin and Sawhney, 1984, Jury et al., 1983, Rapaport, 1985, Scott et al., 1983, USEPA (1985,1986)). Certain biological reactions might be enhanced and, thereby, accelerate biodegradation of the contaminants.

Retention time of water in aquifers may be exceedingly long and almost no studies on long-term transformations of the more biologically reacting materials in aquifer systems are available (McCarthy et al., 1981).

Within such long-term time frames, chemical and biological processes may transform trace organic compounds into materials that are potentially hazardous, the processes involved have not been clearly elucidated.

More information on the relative roles of chemical and biological factors and on the effects of aquifer materials and environments on reaction rates is certainly needed if the long-term fate of trace organic materials in aquifer systems is to be well understood.

The ultimate fate of organic compounds in the subsurface system depends greatly upon their biodegradibility. Available evidence indicates that there is a minimum concentration to which a single organic material can be decomposed under steady state conditions. Thus, concentration is a function of growth and decay coefficients of the microorganisms, which in turn are functions of environmental variables that include i) temperature, ii) pH, iii) bacterial species, and iv) available electron acceptors. An extensive study of the effects of such environmental variables on the ultimate fate and movement of organic materials that enters the subsurface environment is still incomplete and should receive the attention of researchers.

There is ample evidence that trace organic contaminants interact with soil solids and micro-organisms during artificial recharge. Sorption retards solute transport, whereas both sorption and dispersion attenuates concentration fluctuations. Long solute residence time due to sorption coupled with low hydraulic velocities , together with the high specific surface area of porous medium, affords unusual opportunities for microbial growth and biodegradation.

Degradation rate, whether chemical or biological, is highly dependent on molecular structure and environmental conditions. At present, our ability to predict degradation rate is largely unsatisfactory. In-situ experiments or appropriate laboratory models are needed to assess the likelihood of such degradations. Accurate and efficient modeling of subsurface biological processes is a growing area of research today.

4. Although considerable effort has been expended to determine aquifer parameters (permeability and dispersion) experimentally, most studies are made under ideal laboratory conditions and using simplified assumptions. Few studies have been reported in literature which consider the effects of different factors such as contaminant concentration and chemical properties. Some organic chemicals contained in industrial impoundments were found to increase the permeability of clay liners destructively, leading to greater leakage from the impoundments. It has also been reported in literature that the permeability of sedimented muds in pond system is controlled by the presence of chemicals in the voids of the materials and that permeability fluctuates with changes in temperature and the chemical concentration of the pond water. Further, the transport of solute in groundwater is complicated by the effects of low or high permeability lenses due to advection and hydrodynamic dispersion processes which are strongly dependent on groundwater velocities and which are, in turn, influenced by permeability changes.

Because permeability is a function of the medium void ratio and fluid viscosity, any changes in these two properties will change the permeability and, in turn, will affect the transport process. A study of the chemical and biological reactions on the permeability of aquifer materials would be a valuable contribution which would help in modeling solute transport in groundwater. A study of the effects of the environmental variables (temperature, pH,Bio Species) and the concentration of contaminants on aquifer properties such as permeability and dispersion, would yield some understanding of the existing discrepancies between field and laboratory values of such parameters.

5. A variety of solute transport models are presently available. Although a few comparison has been carried out (USEPA, 1988), a systematic comparison of all existing models and the advanced solution techniques would undoubtedly contribute to the development of a more accurate, efficient and reliable model.

6. Many solute transport models reported in the literature do not consider all the probable processes involved. In particular, very few models are available which considered biological processes in their formulation. An efficient model, including the biological processes, is necessary.

7. Further research is needed to obtain a better understanding of reaction rates in the subsurface environment for the coupling

chemical reactions into the transport formulation of the processes.

Chapter - III

MODELING OF GROUNDWATER FLOW AND CONTAMINANT TRANSPORT IN POROUS MEDIA

Chapter - III

MODELING OF GROUNDWATER FLOW AND CONTAMINANT TRANSPORT

3.1 GROUNDWATER CONTAMINATION

3.1.1 Definition:

Groundwater contamination may be defined as the addition of elements, compounds and/or pathogens to water that alters its composition to make it unsuitable for domestic consumption and may be hazardous for the desired purpose.

3.1.2 Sources of Groundwater Contamination:

There are three main sources of groundwater contamination:

1. **Groundwater contamination due to natural processes:**
    - a) Mineralization resulting from leaching
    - b) Evapotranspiration which increases concentration of salts in the remaining water
2. **Groundwater contamination due to man's waste-disposal practices.**
    - a) Individual sewage disposal systems
    - b) Land disposals of solid wastes
    - c) Collection,disposal and treatment of municipal wastewater

d) Industrial and other wastewater impoundments

e) Land spreading of sludge

f) Brine disposal associated with the petroleum industry

g) Disposal of mine wastes

h) Deep-well disposal of liquid wastes

i) Disposal of animal feedlot wastes

j) Disposal of high and low-level radioactive wastes resulting from a variety of activities

3.Groundwater contamination due to human activities but unrelated to waste disposal practices:

a) Accidental spills and leaks

b) Agricultural activities

c) Mining

d) Highway de-icing salts

e) Atmospheric contaminants and acid rains

f) Surface water

g) Improperly planned groundwater development leading to saltwater intrusion.

h) Improper well construction and maintenance.

3.1.3 Applications

The practical applications of dispersion and diffusion phenomena in porous media are as follows:

1. Pollution/Contamination Studies in Groundwater
2. Aquifer Management and Reclamation
3. Salt Intrusion Problems in Coastal Aquifers
4. In situ Study of the Characteristics of an Aquifer
5. Oil Recovery
6. Landfill Investigations

3.2 CLASSIFICATION OF SOLUTES/PERMEANTS

A. Conservative or Nonreacting Solutes
B. Nonconservative or Reactive Solutes
C. Aggressive Solutes

The details of (A) and (B) is available in many standard books on solute transport. The aggressiveness of solute is a new frontier that need to be explored.

3.2.1 Aggressive Solutes

Aggressive solutes may be defined as those solutes which cause a change in the fundamental properties of the porous media when flow of such solutes take place through the medium. A number of solutes exhibiting such property are reported in the related literature. They may be organic or inorganic liquids.

In the context of solute transport in porous media, the effects of such aggressiveness of solutes on the permeability or the hydraulic conductivity are of vital importance. The above definition is related to porous media only.

3.2.2 Solute Aggressiveness

Definition: Solute Aggressiveness may be defined as those properties of a solute or permeant which may cause significant change in physical, chemical and biological properties of the media through which transport of such solutes takes place. It involves a number of mechanisms depending on different factors which are discribed in the following subsections.

3.2.3 Factors Influencing Solute Aggressiveness

The flow and transport of solutes through porous media , being a complex natural phenomena, is influenced by numerous factors. Among them, the following factors may be considered as of much awaited importance especially when solute aggressiveness is concerned.

1. Solute Concentration
2. Solute Composition
3. Soil type and Composition

3.2.4 Mechanisms Involved

According to the potential investigators from the field of Soil science as well as hydrogeology, the following mechanisms are of primary importance in the study of solute aggressiveness in porous media.

1. Clay swelling
2. Clay dispersion
3. Flocculation and/or deflocculation
4. Formation of cracks

Considering the effects of different mechanisms involved with the solute aggressiveness on porous media, it can be concluded that the dramatic changes of hydraulic conductivity of porous media are closely related to the change in porosity of the media (Brawn (1988)).

For example, swelling of clays effects the grain size distribution of the media thereby changing the effective porosity. Swelling of clay particles depends on the solute concentration (Chen (1987)).

Clay dispersion is assumed to cause blocking of fluid conducting pores, but in laboratory experiments (Papusky et.al.(1979)) it was found that eventually it leads to loss of clay in the effluent and to an increase in hydraulic conductivity. If the finer particles are disposed from the sides of the channels of connecting pores, the porosity is increased, thereby causing an increase in hydraulic conductivity.

Flocculation and deflocculation both change the porosity, the increase in the former increases porosity and the increase in the later decreases porosity. Flocculation is also found to be a function of solute concentration (Chen (1987)).

Cracking of the medium due to shrinkage creates channels which contributes to effective porosity of the system and changes the hydraulic conductivity.

From the above discussion, it may be concluded that it may not be critical to study the phenomena of solute aggressiveness in terms of porosity changes which ultimately results in an associated change in a measurable property namely the hydraulic conductivity.

Another advantage of using porosity change as a measure of solute aggressiveness is that the porosity is a macroscopic variable of the medium, which can be modelled using continuum approach.

3.3 MATHEMATICAL EVALUATION OF FACTORS AFFECTING HYDRAULIC CONDUCTIVITY

Hydraulic conductivity is related to the fluid and the medium properties as

$$K = \frac{\kappa g}{\nu} \qquad (1)$$

where

K = hydraulic conductivity

κ = the intrinsic permeability of the medium

g = acceleration due to gravity and

ν = kinematic viscosity of the fluid which is very sensitive to pressure and temperature.

From the above equation, it is clear that K is a function of both the medium and the fluid properties (as κ for the medium and ν for the fluid, g being constant). The solute concentration will definitely change the value of ν.

The following is a careful examination of the effects of κ and ν on the hydraulic conductivity, K .

a) Effect of ν

Let K_0, K, ν_0 and ν be the hydraulic conductivity and the kinematic viscocity at two concentration levels C^0 and$C$ $(C > C_0)$ respectively.

If one considers the common case of Brine (NaCl solution) , for which Hassanizadeh and Leinje (1988) have given the empirical relation between solute mass fraction, density and viscosity.

$$\rho = \rho_0 e^{\gamma\omega + \beta(P-P_0)}$$

where ρ and ρ_0 are the fluid densities at ω and ω_0 solute mass fractions respectively, $\gamma = 0.6923$ for brine $\beta = 10^{-10}$ and $(P-P_0)$ is the thermodynamic pressure. For isothermal condition, we have

$$\frac{\rho}{\rho_0} = e^{\gamma\omega} \tag{a}$$

The fluid viscosity of brine is

$$\mu = \mu_0(1+m(\omega)) \tag{b}$$

$$\text{where } m(\omega) = 1.85\omega - 4.1\omega^2 + 44.5\omega^3 \tag{c}$$

Using the relation $\nu = \frac{\mu}{\rho}$, we have

$$\frac{\nu}{\nu_0} = \frac{\frac{\mu}{\mu_0}}{\frac{\rho}{\rho_0}} = \frac{1+m(\omega)}{e^{\gamma\omega}} \tag{d}$$

Since

$$\frac{K}{K_0} = \frac{\kappa}{\kappa_0}\left(\frac{\nu_0}{\nu}\right) \tag{e}$$

But $\frac{\nu_0}{\nu} < 1.0$ and $\frac{K}{K_0} > 1.0$ for brine where $C > C_0$.

Equation (c) indicates that an increase in solute concentration causes a decrease in hydraulic conductivity which is opposite to the phenomemon of solute aggressiveness of brine i.e. increase of K with concentration.

Therefore, the increase in hydraulic conductivity is certainly associated with the increase in the intrinsic permeability of the medium. Furthermore, the effect of ν on hydraulic conductivity is not so significant (figure-3.1) unless the temperature and pressure play important role.

b) Effect of κ on hydraulic Conductivity

The intrinsic permeability κ, depends on the medium properties, namely

i) porosity (η)
ii) specific surface $S = f(\eta)$
iii) Tortuosity $f(\eta)$ and
iv) the shape factor m .

The ranges of tortuosity and the shape factor are reported to be $0.56 < \text{tortuosity} < 0.80$ and $0.5 < m < 0.6667$ (Bear,1972) respectively. The worst combination of the product of tortuosity and the shape factor (i.e. maximum tortuosity times maximum shape factor $= 0.8(0.6667) = 0.53$ and minimum tortuosity times minimum m $= 0.56(0.5) = 0.28$) can cause a maximum change in κ of about 2 times which is much lower than the change reported in the literature (upto 180 times, Frenkel et.al.(1978), Appendix-A2).

It can be concluded from the above analyses that even in the extreme cases, the two other factors, namely the porosity and the specific surface change with a significant change in the intrinsic permeability.

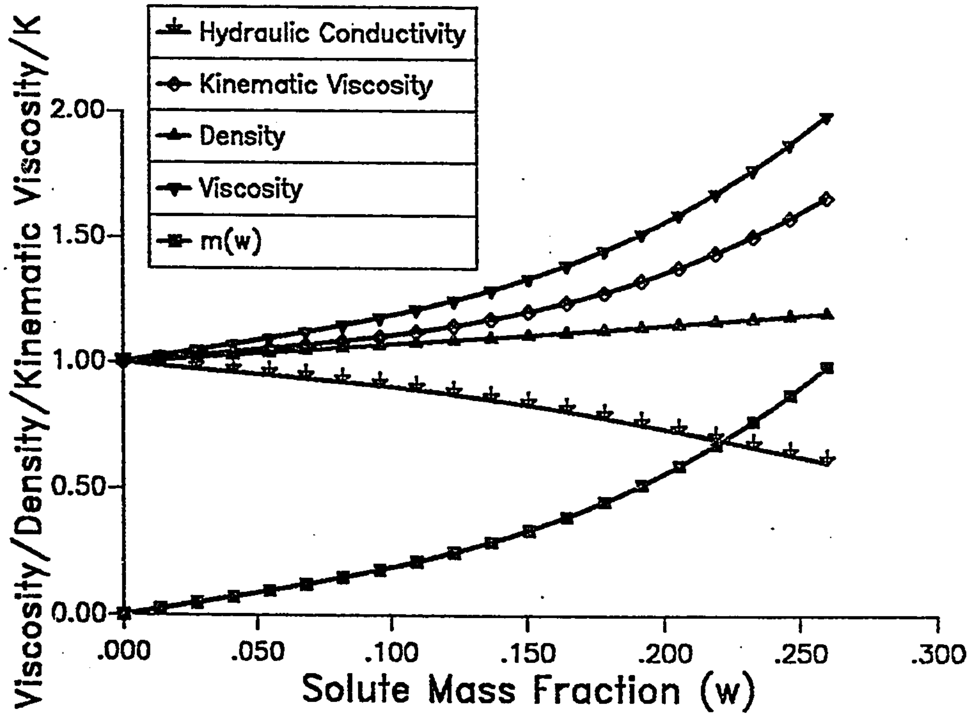

Figure-3.1 : Effect of solute concentration on viscosity, density, and hydraulic conductivity of Brine

3.3.1 Relation Between Hydraulic Conductivity and Porosity

The hydraulic conductivity of porous media pertains to the ease with which a fluid, termed as permeant or solute, passes through the porous materials. It depends on the properties of both porous medium and the solute. The property of the medium which governs the flow is the size of the pores and voids. The governing solute properties are viscosity, the specific weight and the aggressiveness in case of aggressive solutes. Viscosity controls the shear resistance and the specific weight controls the driving forces of the fluid. The effect of solute aggressiveness is to cause a change in medium properties, thereby changing the hydraulic conductivity.

Permeability, sometimes refered to as intrinsic permeability, on the other hand, is independent of fluid properties like viscosity but depends on the medium properties as well as solute aggressiveness.

The relationship between hydraulic conductivity and permeability is expressed mathematically as ;

$$K = \frac{\kappa g}{\nu} \qquad (1)$$

K : hydraulic conductivity

κ : permeability depends

: on size and shape of the pores in soil

: size and shape of soil are influenced by the interaction between soil and percolating solution.

g : gravitational constant

ν : kinematic viscosity $= \frac{\mu}{\rho}$

To define κ as a function of porosity, a relationship that was presented by Kozeny and later developed by Carmen is used . The relationship is based on Poiseulle's law and has been frequently applied in industrial filtration.

For continuous viscous flow through unconsolidated and unstructured granular media in which the pores are not too large, uniform size, evenly distributed and not subject to solute aggressiveness effects like swelling, flocculation, cracking, shrinkage etc., the Kozeny-Carmen equation is

$$\kappa = \frac{\eta^3}{mt^2 S_0^2 (1-\eta)^2} \tag{2}$$

m empirical factor 'm' represents shape and size of particles, η represents the total pore fraction of the medium ,

t represents the tortuosity of the flow path, which is a measure not only of the length of path, but also of the pore-cross-section involves in flow, it enters as a quadratic function,

S_0 represents the specific surface of the soil particles

S specific surface of the flow bed (solution exposed surface area after packing per cm^3 of flow bed and is not directly measurable)

From the above definition of S , it follows that

$$S = S_0(1-\eta) \tag{3}$$

Then

$$\kappa = \frac{\eta^3}{mt^2S^2} \tag{4}$$

The ratio $\frac{\eta}{S}$ implicit in equation (4) is equal to the ratio of pore volume over surface per unit volume of flow bed which accounts for possible noncircularity of pores. Product ' mt^2' is known as Kozeny- Carmen Constant.

Because the shape, tortuosity and the surface of pores are clearly interdependent characteristics of the flow path, the product ' mt^2S^2 ' can be contracted to F^2 which can be later refered to as ' flow matrix factor ' which typifies the morphology and onsuing resistivity of the flow path. Then

$$\kappa = \frac{\eta^3}{F^2} \tag{5}$$

when $F^2 = mt^2S^2$

3.4 RELATION BETWEEN HYDRAULIC CONDUCTIVITY AND SOLUTE AGGRESSIVENESS

Literature survey amply demonstrates the fact that the hydraulic conductivity of porous media depends on the concentration and composition of aggressive permeants. These aggressive solutes cause changes in the morphology and resistivity of the flow path through different mechanisms like swelling, flocculation-deflocculation, cracking, shrinkage etc.

In the following derivation of the relationship between the hydraulic conductivity and solute aggressiveness, recognition will be given to the fact that the aggressiveness of solutes may cause a change in porosity or more specifically in effective porosity through different mechanism which, ultimately exhibits a dramatic change in the hydraulic conductivity of the soil.

If it is assumed that subtraction of the change of porosity due to solute aggressiveness from the total porosity yields the porosity that permits unhindered flow , then

$$\kappa = \frac{(\eta - \Delta\eta)^3}{mt^2 S_0^2 (1 - (\eta - \Delta\eta))^2} \qquad (6)$$

where ($\eta - \Delta\eta$) is the effective porosity .

If a soil is percolated with an aggressive solute of two different concentrations, i and j , we can write from equation (5)

$$\frac{\kappa_i}{\kappa_j} = \frac{\eta_i^3}{\eta_j^3}\left(\frac{F_j^2}{F_i^2}\right) \tag{7}$$

where

η_i = the effective porosity at concentration i

η_j = the effective porosity at concentration j

κ_i = permeability at concentration i

κ_j = permeability at concentration j

$$F_i^2 = mt_i^2S_i^2 = mt_i^2S_0^2(1-\eta_i)^2 \tag{8}$$

$$F_j^2 = mt_j^2S_j^2 = mt_j^2S_0^2(1-\eta_j)^2 \tag{9}$$

The ratios $\frac{\eta_i}{\eta_j}$ and $\frac{F_i}{F_j}$ denote factors by which the porosity and the flow matrix change when the solute concentration is changed from i to j .

For hydraulic conductivity, we have from equation (1)

$$K_i = \frac{\kappa_i g}{\nu_i} \tag{10}$$

$$K_j = \frac{\kappa_j g}{\nu_j} \tag{11}$$

therefore from equation (10) and (11)

$$\frac{K_i}{K_j} = \frac{\kappa_i}{\kappa_j}\left(\frac{\nu_j}{\nu_i}\right) \tag{12}$$

As the solute aggressiveness changes with the concentration, there should be a resulting change in tortuosity and also in pore surface. As defined earlier,

$$F^2 = mS_0t^2(1-\eta)^2 \tag{13}$$

If we express $t^2 = f_1(\eta)$,and $(1-\eta)^2 = f_2(\eta)$ then,

$$F^2 = mS_0f_1(\eta)f_2(\eta) \tag{14}$$

Or $F^2 = (mS_0)F(\eta)$

where $F(\eta) = f_1(\eta)f_2(\eta)$

If we study the behavior of $F(\eta)$, qualitatively considering the phenomena involved in $f_1(\eta)$ and $f_2(\eta)$ then it is evident from figure-3.2 that $f_2(\eta)$ decreases as η increases in the realistic range of η for a porous media i.e. $0 < \eta < 1.0$.

On the otherhand, $f_1(\eta)$ can be defined as a function of η satisfying the tortuosity conditions for two extreme conditions ,namely

i) at $\eta = 0$, the tortuosity is undefined

ii) at $\eta = 1.0$, the tortuosity value is unity, as in the case of pure fluid flow.

A convenient qualitative functional representation of $f_1(\eta)$ satisfying the above two conditions is

$$f_1(\eta) = \frac{1}{\eta^r} \text{ for } r > 0 . \tag{15}$$

The qualitative variation of $f_1(\eta)$ is shown in figure-3.3 for different values of r.

Based on the above definitions of $f_1(\eta)$ and $f_2(\eta)$, the qualitative nature of $F(\eta)$ is shown in the figure-3.4. Under these condition, we have from (14) and (15),

$$F_i^2 = mS_0 \frac{1}{\eta_i^r}(1-\eta_i)^2 \tag{16}$$

and

$$F_j^2 = mS_0 \frac{1}{\eta_j^r}(1-\eta_j)^2 \tag{17}$$

If we take the ratio of equations (16) and (17)

$$\frac{F_i^2}{F_j^2} = \frac{\eta_j^r}{\eta_i^r} \frac{(1-\eta_i)^2}{(1-\eta_j)^2} \tag{18}$$

Then, we have from (7) and (18),

$$\frac{\kappa_j}{\kappa_i} = \frac{\eta_j^3}{\eta_i^3} \frac{\eta_j^r}{\eta_i^r} \frac{(1-\eta_i)^2}{(1-\eta_j)^2}$$

$$\text{Or } \frac{\kappa_j}{\kappa_i} = \frac{\eta_j^{3+r}}{\eta_i^{3+r}} \frac{(1-\eta_i)^2}{(1-\eta_j)^2} \tag{19}$$

The above equation expresses the relation between the relative permeability and the porosity for aggressive solutes. Figure-3.5 is obtained by solving the above equation for the porosity factor $\frac{\eta_j}{\eta_i}$ for a given value of $\frac{\kappa_j}{\kappa_i}$. Newton-Rapson method is used to solve this nonlinear eqation (Appendix-B2).

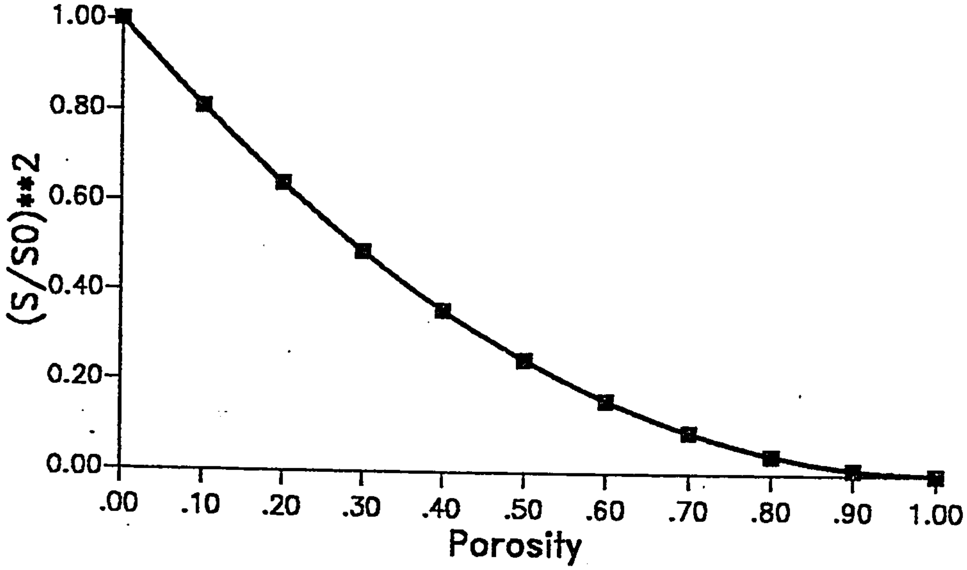

Figure-3.2 : Porosity and specific surface relationship in porous media

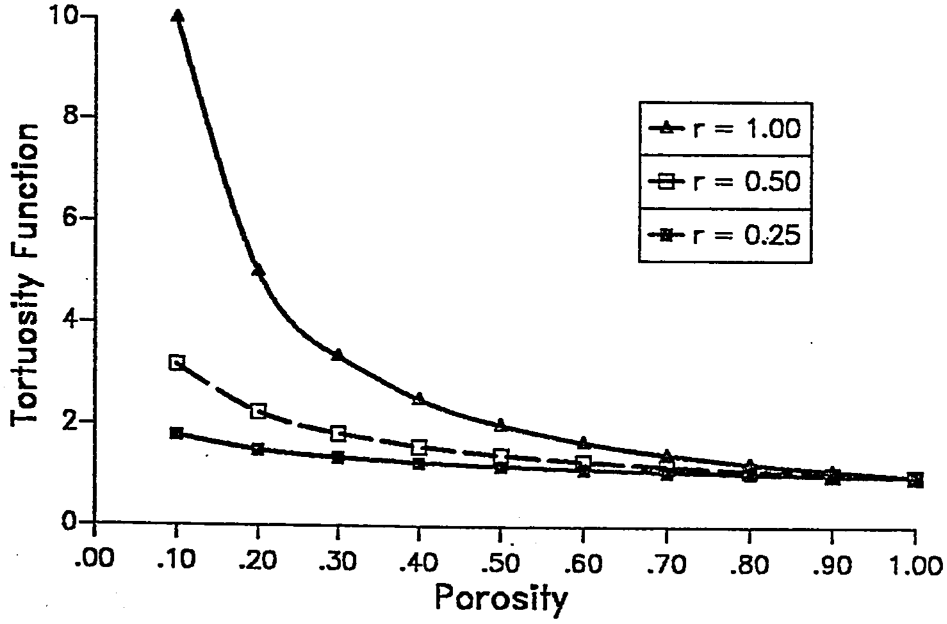

Figure-3.3a : Porosity and tortuosity relationship in porous media (for r = 0.25, 0.50 and 1.0)

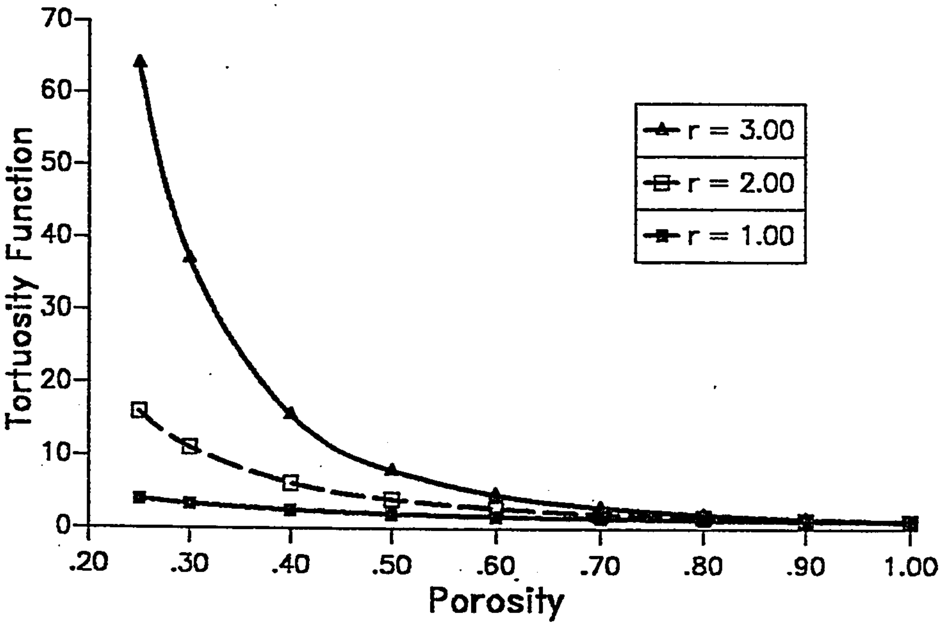

Figure-3.3b : Porosity and tortuosity relationship in porous media (for r = 1.00, 2.00 and 3.0)

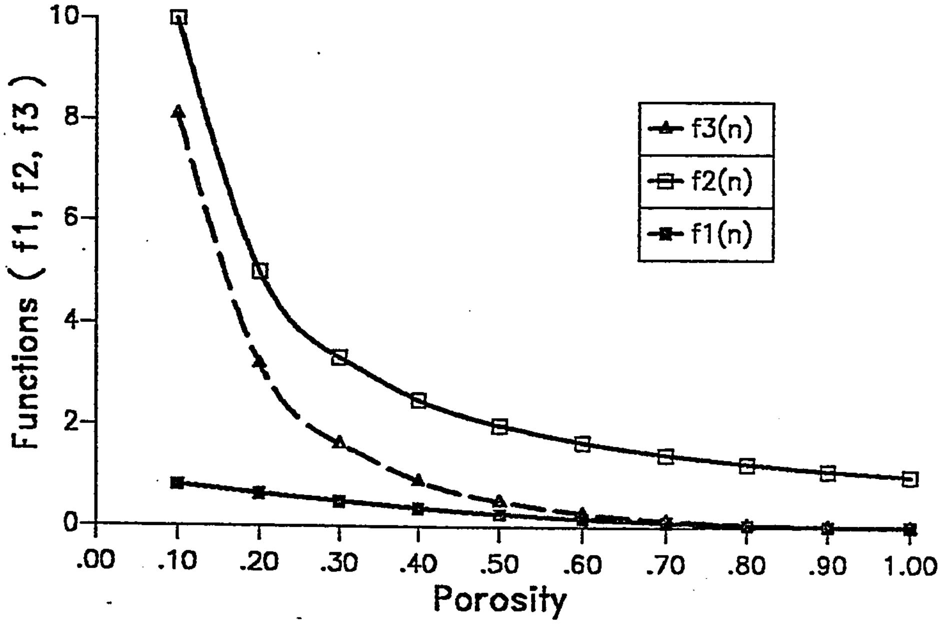

Figure-3.4 : Graph of functions $f_1(\eta)$, $f_2(\eta)$, and $f_3(\eta)$

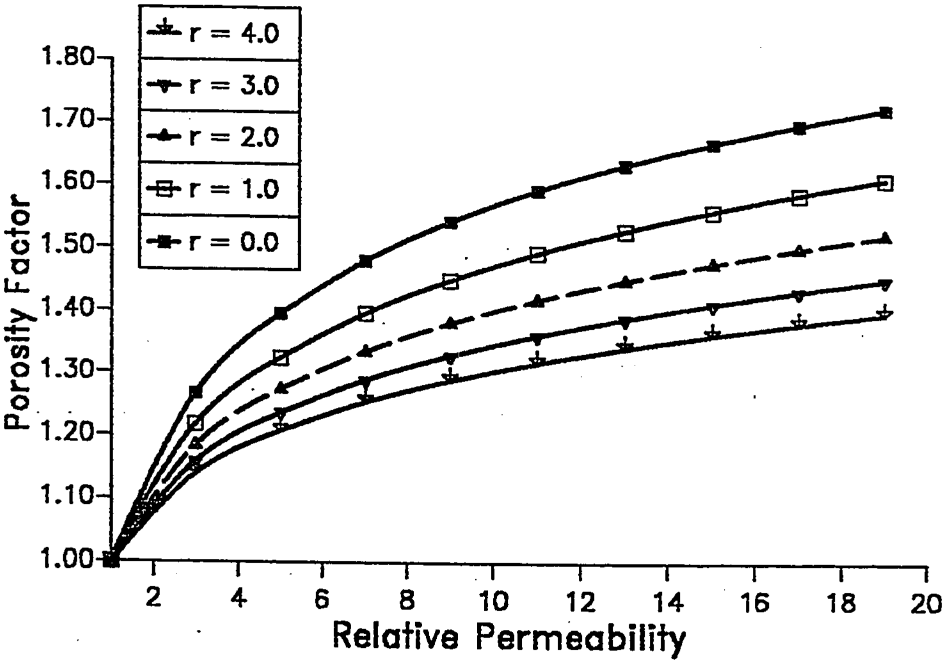

Figure-3.5a: Porosity and permeability relationship in porous media satisfying Kozeney-Carman equation (for initial porosity = 0.40)
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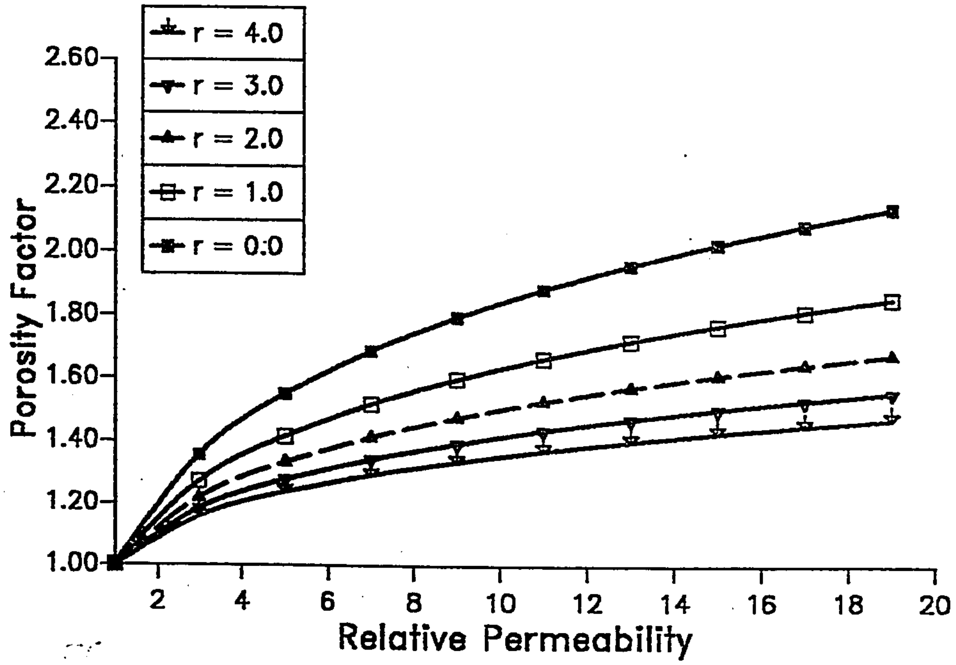


Figure-3.5b: Porosity and permeability relationship in porous media satisfying Kozeney-Carman equation (for initial porosity = 0.20)

An alternative approach to eliminate the ratio of flow matrix factors ,specially in case when clay swelling is dominant, is to assume that the resultant changes are proportional to the effective porosity changes in the following general form:

$$[\frac{F_i}{F_j}]^2 = [\frac{\eta_i}{\eta_j}]^s \qquad (20)$$

where 's' is any exponent the value of which depends on the degree of aggressiveness caused by the permeants.

Under this assumption and from (7) and (20),

$$\frac{\kappa_i}{\kappa_j} = \frac{\frac{\eta_i^3}{F_i^2}}{\frac{\eta_j^3}{F_j^2}} = \frac{\eta_i^3}{\eta_j^3}\frac{F_j^2}{F_i^2} \qquad (21)$$

Substitution of the above proportionality relation (20) into (21), we obtain

$$\frac{\kappa_i}{\kappa_j} = (\frac{\eta_i}{\eta_j})^{(3-s)} \qquad (22)$$

Considering the equations above , we may conclude that the permeabilities are proportional to the effective porosities elevated to a power , say 'p' where p = (3-s). To determine the range of 'P', consider the following four cases;

Case -I : s = 0 which indicates that the net effect of porosity change on the flow matrix factor, F ,is negligible, then p = 3 in equation (22).

Case -II : s = 3 , for which p = 0 which indicates that the net effect of porosity change on permeability is negligible i.e. the case of non-aggressive solutes.

Case -III : $s < 0$, say -1, for which $p > 3$ and

$$[\frac{F_i}{F_j}]^2 = [\frac{\eta_i}{\eta_j}]^{-1}$$

or $$[\frac{F_i}{F_j}]^2 = [\frac{\eta_j}{\eta_i}]$$

which indicates that the flow matrix factor is inversely proportional to porosity. This is opposite to the assumption made earlier pertaining to soil change due to swelling .

Case -IV : $s > 3$, say 4, for which $p < 0$ i.e $p = -1$ from equation (22),

$$\frac{\kappa_i}{\kappa_j} = (\frac{\eta_i}{\eta_j})^{-1}$$

or

$$\frac{\kappa_i}{\kappa_j} = \frac{\eta_j}{\eta_i}$$

which indicates that the permeability is inversely proportional to porosity .

Situation IV above is clearly unrealistic in any soil model, while case III is incompatible for a realistic soil model, then p should be in the range $0 < p < 3$.

When $0 < p < 3$, it could be construed to indicate that F remains neither constant, nor changes by a factor causing κ to remain constant when concentration is changed from i to j in the percolating sequence.

Summarizing, we have

$$\frac{\kappa_j}{\kappa_i} = \frac{\eta_j^{3+r}}{\eta_i^{3+r}} \frac{(1-\eta_i)^2}{(1-\eta_j)^2} \qquad (19)$$

Or

$$\frac{\kappa_i}{\kappa_j} = [\frac{\eta_i}{\eta_j}]^p \qquad (23)$$

From the relation,

$$\frac{K_i}{K_j} = \frac{\kappa_i}{\kappa_j}(\frac{v_j}{v_i}) \qquad (12)$$

we have

$$\frac{K_i}{K_j} = (\frac{v_j}{v_i})(\frac{\eta_i}{\eta_j})^p \qquad (24)$$

where $0 \leq p \leq 3$.

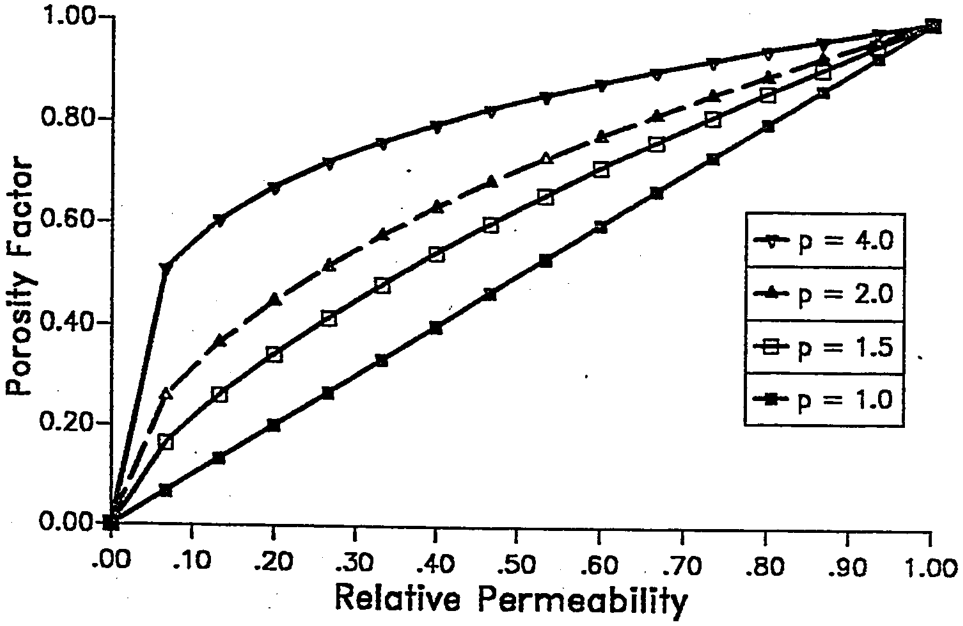


Figure-3.6a : Porosity and permeability relationship in porous media for swelling dominated case

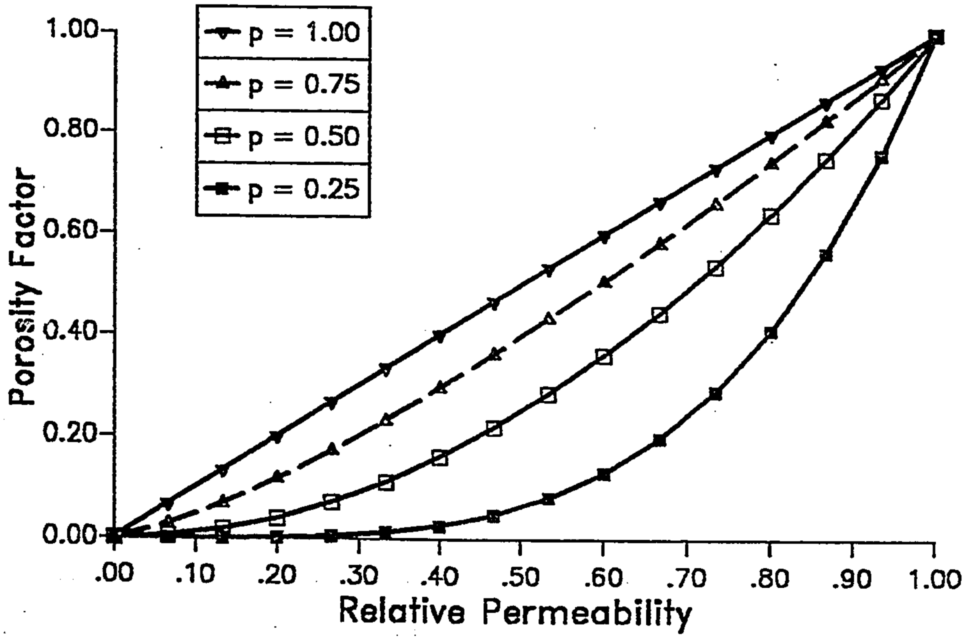


Figure-3.6b : Porosity and permeability relationship in porous media for swelling dominated case

$$\frac{K_j}{K_i} = \frac{v_i}{v_j}\frac{\eta_j^{3+r}}{\eta_i^{3+r}}\frac{(1-\eta_i)^2}{(1-\eta_j)^2} \text{ for } r > 0 . \tag{25}$$

Equations (24 and 25) describe the relative hydraulic conductivity of a soil which is first percolated with a solution of concentration i and subsequently with another concentration j , differing mainly in aggressiveness it causes.Therefore, these equations express the relationship between the hydraulic conductivity and the solute aggressiveness in terms of effective porosity. These equations may be used to evaluate the additional terms appearing in the flow and the transport equations (as given by equations (26) and (42), respectively) for aggressive solutes namely;

$$\left(\frac{\partial \eta}{\partial t}\right)_{s.a.} \text{ and } \frac{\partial \eta}{\partial x_j}$$

The above equations are also conformable with the Kozeny-Carmen equation when the viscosity and the density effects as well as the solute aggressiveness is neglected i.e. for $v_i = v_j$ and $K_j = K_i$ or $\eta_i = \eta_j$,from equations (24) and (25),

$$\frac{K_i}{K_j} = 1 \text{ or } K_i = K_j = K \text{ for non-aggressive solutes or permeants.}$$

It is interesting to observe that the nature of relative permeability variations in both equations are similar although the assumptions for the flow matrix factors are contradictory. This similarity supports the finding that the combined effect of flow matrix factors on the relative permeability and porosity is insignificant. Thus p = 3 and the expression is very simple. It may be also true that the interaction of different mechanisms may role out the effect of the flow matrix factor.

Equations (24) and (25) is applicable to the soil models which satisfy Kozeny-Carmen equation. If the intrinsic permeability is expressed as a function of effective grain diameter, expressions are required to define effective grain diameter, solute concentration and porosity relationship. Since no such relationship exists, one way to deal with this problem is to solve the governing equations for concentration-dependent parameters simultaneously, neglecting the heterogeneity due to porosity change.

3.5 MODELING OF AGGRESSIVE SOLUTE TRANSPORT

The major factor to be considered in modeling aggressive solute transport in porous media is that any change in the properties of the media induced by the solute percolation should be taken into account properly.

For example, in the modeling of solute transport in porous media, for both conservative and nonconservative solutes, the medium properties like porosity, hydraulic conductivity , hydrodynamic dispersion is assumed to be independent of solute concentrations which makes the governing equations linear. But in the case of aggressive solute transport, the resulting equations are nonlinear due to the change of medium properties that are affected by solute concentration.

It should also be noted that these concentration-dependent parameters are completely different from the density-dependent nonlinear problems of solute transport phenomena. Because, in the latter case, the property changes in the medium is not taken into consideration. Furthermore, the simulation or the prediction model of aggressive solute transport requires the solution of a coupled system of groundwater flow and the transport equations.

Secondly, the validity of the assumptions made in the case of non-aggressive solute transport problems are questionable in the case of aggressive solutes. Some of these are discussed below.

1. assumption of constant porosity η in the formulation is not valid since its change causes changes in the model parameters.
2. Any change in medium properties results in losses of

homogeneity in the case of concentration-dependent model parameters.

3. the assumptions made at low concentrations are not applicable because the solute aggressiveness may be significant at high concentrations.
4. the condition of incompressible unsteady flow may exist when $\frac{\partial \rho}{\partial t} = 0$ and $q.\mathrm{grad}\rho = 0$ in case of a nondeformable porous media. When the solute is aggressive, $(\frac{\partial \eta}{\partial t})_{s.a.}$ component along with the term related to induced heterogeneity in the flow equation introduces the concept of incompressible unsteady flow situation for a nondeformable media.
5. the solution algorithm needs to be capable of solving simultaneously, the groundwater flow equation and the transport equation (both developed for variable porosity and considering solute aggressiveness).

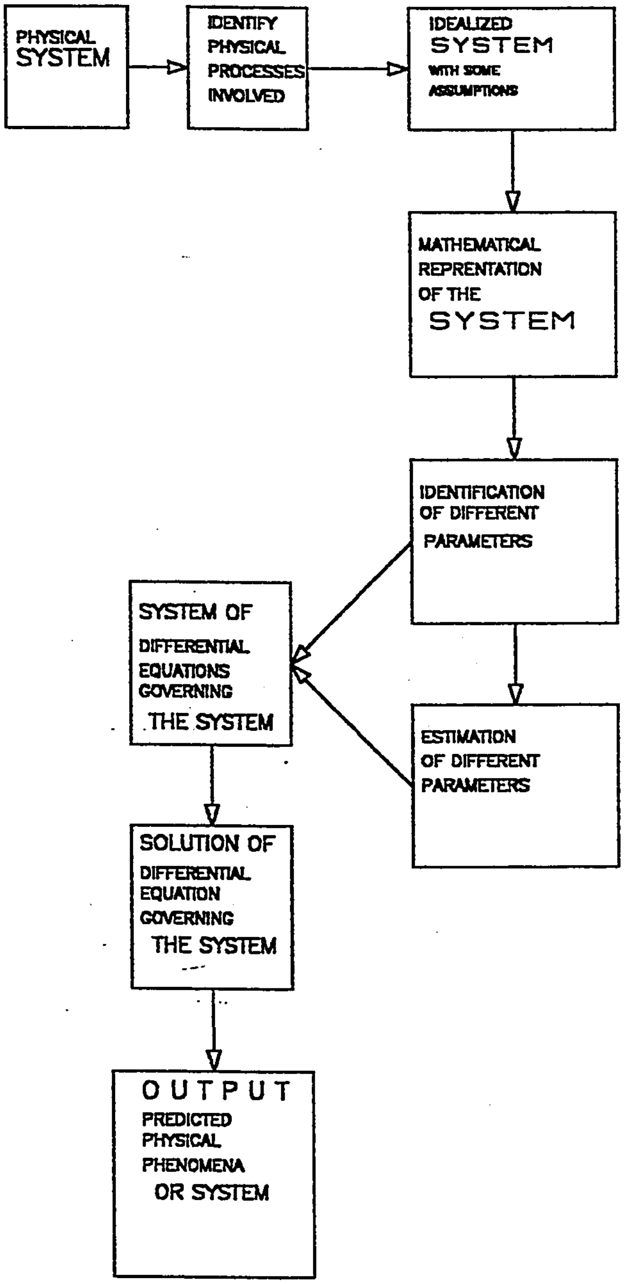


Figure-3.7 : Summary of basic concepts of modeling scientific problems

3.6 FORMULATION OF THE GOVERNING EQUATIONS

The formulation of the governing equations for aggressive solute transport problems needs careful examination of different conventional practices and assumptions for solute transport problems. As mentioned earlier, the aggressive solutes are those solutes(organic and/or inorganic salts) which changes the property of the media when flow of such solutes take place in any media. The most fundamental property of special interest is the hydraulic conductivity of the media, on which significant change is reported in the literature.

Looking at different factors influencing hydraulic conductivity or the permeability of the media, and the related mechanisms of solute aggressiveness on the media, the change in medium porosity seems to be considered first.

The modification of the governing equations proposed here are based on the following considerations.

i) Formulations should be done for a variable porosity, thereby a heterogeneous medium

ii) porosity change will be taken into consideration in the process of averaging over the Representative Elementary Volume (REV).

iii) The formulation is based on the procedure followed by Bear (1972) and Konikow and Grove (1977).

iv) Detail derivation is not repeated here, instead, the importance of different terms are discussed in the light of present literature.

3.6.1 Groundwater Flow Equation

The familiar form of the continuity equation is :

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = \frac{\partial(\rho\eta)}{\partial t}$$

$$\text{or } \frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = \eta\frac{\partial \rho}{\partial t} + \rho\frac{\partial \eta}{\partial t} \qquad (26)$$

The conventional practices to evaluate the right hand side of this equation are:

1. Assuming nondeformable media and/or incompressible fluid in which case the right hand side becomes zero ; resulting with incompressible unsteady flow condition i.e steady head distribution only.
2. To relate $\frac{\partial \rho}{\partial t}$ and $\frac{\partial \eta}{\partial t}$ with deformation to obtain storage coefficient $S = \rho^2 g[\alpha(1-\eta)+\beta\eta)]$ (Appendix-B3) and the term $\frac{\partial h}{\partial t}$
3. Treating η as constant.

Bear (1972) introduced two types of porosity, namely;

a) original porosity - formed during the formation of the medium
b) induced porosity - induced later and due to geophysical changes and/or some chemical reactions.

Bear (1972) did not mention the later type of porosity change that is due to solute aggressiveness. If the porosity induced by solute aggressiveness is considered , it may not be sufficient to relate $\frac{\partial \eta}{\partial t}$ with the deformation of the media. Because the mechanisms of solute aggressiveness i.e. swelling, dispersion, shrinkage, flocculation or deflocculation may induce porosity without any appreciable deformation. Furthermore, the induced porosity due to solute aggressiveness being a function of solute concentration, is time dependent in transient transport problems. In other words, the induced heterogeneity is transient as long as the concentration distribution remains transient. Therefore, it appears appropriate to split the term $\frac{\partial \eta}{\partial t}$ into two components,

a) $(\frac{\partial \eta}{\partial t})_{def}$ = change of porosity with deformation of the media

b) $(\frac{\partial \eta}{\partial t})_{s.a}$ = change due to solute aggressiveness without deformation.

It should be noted here that $\frac{\partial \rho}{\partial t}$ is assumed to be independent of solute aggressiveness since no such information is available yet. Since any change in solute concentration and/or medium deformation causes change in ρ, $\frac{\partial \rho}{\partial t}$ may be written as two components,

1) $(\frac{\partial \rho}{\partial t})_{def}$ = change of density with deformation of the media

2) $(\frac{\partial \rho}{\partial t})_{\text{Conc.}}$ = change of ρ due to solute concentration

Since $(\frac{\partial \rho}{\partial t})_{\text{conc.}}$ has no significant effect on groundwater flow, it is usually neglected.

The justification of the above analogy is discussed mathematically with reference to the groundwater flow equation.

Assume first that the change of η is only related to deformation or compressibility of the medium and the fluid. Then the groundwater flow equation becomes

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = S\frac{\partial h}{\partial t} \tag{27}$$

where the change of η due to deformation is considered in S. Therefore , this equation cannot describe the accurate flow phenomena of aggressive solutes.

Secondly, if we assume homogeneous incompressible fluid and nondeformable media , then S = 0, which reduces the flow equation (27) into

$$\frac{\partial}{\partial x_i}(K_{ij}\frac{\partial h}{\partial x_j}) = 0 \tag{28}$$

It is interesting to note that in above case, the unsteady flow does not exist. But the porosity change due to solute aggressiveness ,when not associated with deformation, makes the flow field unsteady even in the case of incompressible fluid and media. Mathematically,

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = \eta(\frac{\partial \rho}{\partial t})_{def} + \rho(\frac{\partial \eta}{\partial t})_{def} + \rho(\frac{\partial \eta}{\partial t})_{s.a.} + \eta(\frac{\partial \rho}{\partial t})_{Conc} \qquad (29)$$

or $$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = [\eta\frac{\partial \rho}{\partial t} + \rho(\frac{\partial \eta}{\partial t})_{def}] + \rho(\frac{\partial \eta}{\partial t})_{s.a.} + \eta(\frac{\partial \rho}{\partial t})_{Conc} \qquad (30)$$

For low solute concentration, $(\frac{\partial \rho}{\partial t})_{Conc}$ becomes insignificant and we get,

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = S\frac{\partial h}{\partial t} + \rho(\frac{\partial \eta}{\partial t})_{s.a.} \qquad (31)$$

when $S = 0$ and K_{ij} depends on time, equation (31) reduces to

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = \rho(\frac{\partial \eta}{\partial t})_{s.a.} \qquad (32)$$

The equation (32) above clearly indicates the existence of incompressible unsteady flow for the case of aggressive solute transport problems.

If the solute aggressiveness is considered to be an irreversible process, then the pseudotransient or pseudo-unsteady incompressible flow exists i.e. porosity change for the first arival of the solute is to be considered in case of irreversible aggressiveness. In this case the transient behavior of the medium properties follows the tracer movement.

3.6.2 General Equation of Hydrodynamic Dispersion

The equation describing the three-dimensional Transport and dispersion of a dissolved solute in the flowing groundwater can be derived from the principle of conservation of mass (continuity equation). The general equation presented here is derived on the basis of the developments of Bear (1972) and Konikow (1977).

Since the solute aggressiveness appears to introduce a new concept of incompressible unsteady flow, the modeling of such solute transport problem needs careful formulation of the equation of hydrodynamic dispersion. In addition to the previous concepts, the new concept of solute aggressiveness is emphasized here.

From the mass conservation equation of a solute , averaging over the void space of a REV , we get , from Bear (1972) and Konikow and Grove (1977),

$$\frac{1}{\eta}\frac{\partial(\eta C)}{\partial t}=\frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j})-\frac{\partial}{\partial x_i}(Cv_i)-\frac{Cv_i}{\eta U_0}\frac{\partial(\eta U_0)}{\partial x_i}+\frac{D_{ij}}{\eta U_0}\frac{\partial C}{\partial x_j}\frac{\partial(\eta U_0)}{\partial x_i}+M \quad (37)$$

where 'M' represents additional terms if any .

From the third and fourth terms of the above equation , we have $\eta \neq$ constant for the aggressive solutes which causes a change in porosity of the media (Brawn 1988).

Expanding

$$\frac{Cv_i}{\eta U_0}\frac{\partial(\eta U_0)}{\partial x_i} = \frac{Cv_i}{\eta U_0}\{U_0\frac{\partial \eta}{\partial x_i} + \eta\frac{\partial U_0}{\partial x_i}\} \quad (38)$$

From the conceptual definition of porous media in context of applicability of continuum approach (Bear (1982)), U_0 = Constant , equation (38) reduces to

$$\frac{Cv_i}{\eta U_0}\frac{\partial(\eta U_0)}{\partial x_i} = \frac{Cv_i}{\eta}\{\frac{\partial \eta}{\partial x_i}\} \tag{39}$$

Similarly , we get

$$\frac{D_{ij}}{\eta U_0}\frac{\partial C}{\partial x_j}\frac{\partial(\eta U_0)}{\partial x_i} = \frac{D_{ij}}{\eta}\frac{\partial C}{\partial x_j}\frac{\partial \eta}{\partial x_i} \tag{40}$$

Substitution of equation (39) and (40) into (37) gives

$$\frac{1}{\eta}\frac{\partial(\eta C)}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(Cv_i) - \frac{Cv_i}{\eta}\frac{\partial \eta}{\partial x_j} + \frac{D_{ij}}{\eta}\frac{\partial C}{\partial x_j}\frac{\partial \eta}{\partial x_i} + M \tag{41}$$

Expanding the first term and rearranging , we get

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(Cv_i) - \frac{Cv_i}{\eta}\frac{\partial \eta}{\partial x_j} + \frac{D_{ij}}{\eta}\frac{\partial C}{\partial x_j}\frac{\partial \eta}{\partial x_i} - \frac{C}{\eta}\frac{\partial \eta}{\partial t} + M \tag{42}$$

Or in vector form ;

$$\frac{\partial C}{\partial t} = \mathrm{div}(D.\mathrm{grad}C) - \mathrm{div}(CV) - \frac{CV}{\eta}.\mathrm{grad}\eta + \frac{1}{\eta}D\mathrm{grad}C.\mathrm{grad}\eta - \frac{C}{\eta}\frac{\partial \eta}{\partial t} + M \tag{42a}$$

The equations (42 and 42a) represent the general equation of hydrodynamic dispersion in flowing groundwater considering the additional process of solute aggressiveness.

3.7 MATHEMATICAL TREATMENT OF SOLUTE AGGRESSIVENESS

Careful observation of the general equation of hydrodynamic dispersion presented above clearly identifies the three additional terms compared to the conventional form. We can define a single parameter to express the three terms together, namely,

$$S_a = \frac{1}{\eta}\{v_i\frac{\partial \eta}{\partial x_j} - \frac{D_{ij}}{C}\frac{\partial C}{\partial x_j}\frac{\partial \eta}{\partial x_i} + \frac{\partial \eta}{\partial t}\} \qquad (43)$$

where S_a is the aggressiveness factor of solute in the transport phenomena.

From the above definition, S_a , depends on the medium heterogeneity and the transient behavior of the medium properties which is in agreement with the recent literature related to solute aggressiveness.

We can further simplify the expression for S_a if we consider the terms $\frac{\frac{\partial C}{\partial x_j}}{C}$ and $\frac{\partial \eta}{\partial x_i}$ to be small enough to neglect their product. S_a then becomes

$$S_a = \frac{1}{\eta}\{v_i\frac{\partial \eta}{\partial x_j} + \frac{\partial \eta}{\partial t}\} \qquad (44)$$

With the above definition of S_a, the general equation of hydrodynamic dispersion (42,43) becomes

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(Cv_i) - S_aC + M \qquad (45)$$

The value of S_a can be evaluated at any point or time if the velocity field and the porosity distribution is known.

3.8 SALIENT FEATURES OF THE FORMULATION

Dropping the term 'M' for the time being, the equations are;

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = S\frac{\partial h}{\partial t} + \rho(\frac{\partial \eta}{\partial t})_{s.a.} \tag{31}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(Cv_i) - S_a C \tag{45}$$

1. The above equations take into account the variation of porosity of the medium due to both deformation and solute aggressiveness.

2. The existing models for heterogeneous medium requires that medium heterogeneity data be constant input parameters and do not incorporate the heterogeneity induced by solute aggressiveness. But in the present formulation,any type of medium heterogeneity can be incorporated as the model parameters and can be considered to be transient or pseudotransient.

3. These equations become conventional equations when the variation of porosity is dropped as in the case of non-aggressive solutes.

4. As a normal practice, other terms that are connected to different processes can be easily included in the transport equation.

5. Unlike the conventional practice of coupling the two equations by density or viscosity terms, they can be coupled by the porosity term and the permeability term since K = f(C).

6. Since aggressive solutes change the permeability of the medium, and since K is a function of concentration ,C, the system is nonlinear which needs to be solved simultaneously.

7. The mathematical definition of the factor S_a is in full agreement with the nature of aggressive solutes as mentioned in the related literature.

Chapter IV

SOLUTION OF THE GOVERNING EQUATIONS

Chapter IV

SOLUTION OF THE GOVERNING EQUATIONS

4.1 SOLUTION METHODOLOGY

Solution of the differential equations governing any physical system and/or phenomenon, is to find the unknown function that satisfy the governing equation with the associated boundary and initial conditions. There are many alternative methods for solving such problems. The wide spectrum of these methods can be broadly classified as analytical and numerical.

Some of the important methods are :

1. **Analytical Methods**
    - a) Separation of variables
    - b) Similarity solutions
    - c) Complex variable techniques
    - d) Fourier and Laplace transformations
    - e) Green functions
    - f) Regular and singular perturbations
    - g) Power series.

2. **Numerical Methods**
    - a) Finite Difference Methods
    - b) Finite Element Methods
    - c) Methods of characteristics.

Various finite element approaches are listed in figure - 4.1.

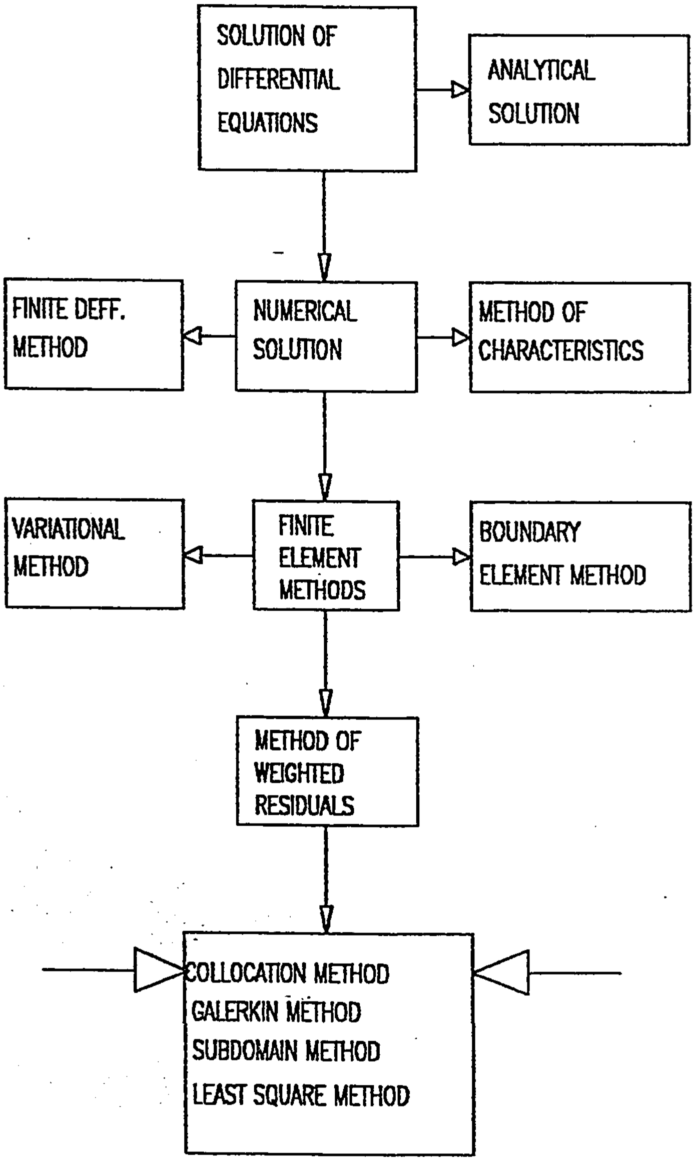


Figure- 4.1 : Summary of solution methods for Differential equations

4.2 ANALYTICAL METHODS

For a number of problems involving linear or quasi-linear equations and regions of simple or regular geometry, it is possible to obtain exact solutions by analytical methods. This is often accomplished by a separation of variables or by applying a transformation that makes the variables separable and leads to a similarity solution. Occasionally, the complex-variable technique, the Green's function approach or a Laplace or fourier transformation of the differential equation leads to an exact solution.

For non-linear problems with regions of regular geometry, very few analytical solutions exist and these are usually approximate solutions obtained by using perturbation or power series method. Because regular and singular perturbation methods are applicable primarily when the non-linear terms in the equation are small in comparison to the linear terms, their usefulness is limited. The power series method is powerful and has been employed with some success, but because the method require evaluation of a coefficient for each term in the series, it is relatively tedious. Also, it is difficult, if not impossible, to demonstrate that the power series converges to the correct solution.

In strict sense, almost all the physical systems are governed by complex non-linear partial differential equations. Problems involving such complex system of non-linear partial differential equations are generally intractable analytically. For such problems, the use of numerical methods to obtain approximate solutions is advantageous.

4.3 NUMERICAL METHODS

The emphasis on solving analytically intractable problems of complex nature to the stage of generating numerical results is deliberate. Because, this underlines the common belief that computation is the total process of problem formulation, mathematical analysis, algorithm development, and the execution of a computer program to obtain the results.

A number of numerical techniques,as mentioned earlier, are available. Some of them are very straight forward and do not require the knowledge of advanced mathematics. The advanced techniques need sound background in advanced mathematics.

Advantages and Disadvantages of Different Numerical Techniques:

1. Finite difference Method

Finite difference method is the most popular numerical approach for simulation of large systems. There are several practical reasons for this popularity. Finite difference methods are conceptually straightforward. The fundamental concepts are readily understood and do not require advanced training in applied mathematics. Moreover, due to their extensive history, they boast a firm theoretical foundation. In addition, because of the form and algebraic simplicity of the equations arising from difference approximations, several clever algorithms have been developed for their solution efficiently. Finite difference method is most suitable for problems with simple or regular geometry. The method becomes complicated and inefficient when the problem is non-linear with irregular domain. The serious drawback of finite difference method is that it becomes very difficult to develop a general purpose computer code for a class of problems with various type of boundary conditions. Most of the formulations are problem oriented.

2. Finite Element Methods:

The application of the finite element method to subsurface problems followed two distinctly different paths. Two basic types of formulations are generally used :

i) formulation based on variational principles

ii) formulation based on the concept of weighted residuals.

The existence of an Euler-Lagrange equation corresponding to the governing equation follows as a necessary condition for the solution of a variational problem.

Unfortunately the converse is not true, that is, the existence of a differential equation does not guarantee the existence of an equivalent variational principle.

The method of weighted residuals is a means to obtain an approximate solution to a differential equation for which the Euler-Lagrange equation may or may not exist.

It does this by requiring that the error between the approximate solution and the true solution be orthogonal to the functions used in the approximation.

4.4 METHODS OF WEIGHTED RESIDUALS

To illustrate the basic concepts of the Methods of Weighted Residuals (MWR), let us consider a differential equation of the form

$$L(u) = f \text{ in } \Omega$$

where, Ω is a bounded domain, L is the differential operator, which acts on the unknown function u to gererate the unknown forcing function.

In finite elements, u is approximated by $\hat{u}(x,y,z)$ which is made up of linear combination of suitable functions (basis/ shape functions) satisfying the essential boundary conditions of the boundary value problem involving unknown coefficients. Then,

$$\hat{u}(x,y,z) \approx u(x,y,z) = \sum_{j=1}^{k} U_j N_j(x,y,z)$$

where

U_j = unknown coefficients to be determined

$N_j(x,y,z)$ = one member of assumed approximation functions for the elements, k corresponds to the number of degrees of freedom for each element in the spatial domain Ω.

Because of the approximation involved, i.e. $\hat{u}(x,y,z) \approx u(x,y,z)$, substitution of $\hat{u}(x,y,z)$ in the differential equation $L(u) - f = 0$, does not satisfy it and we have a residual $R(x,y,z)$ where

$$R(x,y,z) = L(\hat{u}) - f \text{ in } \Omega$$

$R(x,y,z)$ should ideally be zero everywhere in Ω., In the methods of weighted resuduals, the unknown coefficients in describing $\hat{u}(x)$ are obtained by setting the integral of the weighted residual $R(x).W(x)$ to zero, i.e

$$\int_{\Omega} R(x,y,z) W_i(x,y,z) d\Omega = 0$$

where $W_i(x,y,z)$ is a certain weighting function.

The three popular methods of weighted resuduals are the results of the choice of particular weighing function $W_i(x,y,z)$. These are

i) when $W_i(x,y,z) = N_i(x,y,z)$, we have the Galerkin Method.

ii) when $W_i(x,y,z) = 1$ over a subdomain of Ω, we have the subdomain Collocation Method

iii) when $W_i(x,y,z) = \delta(x-x_i)(y-y_i)(z-z_i)$, we have the Collocation Method.

4.4.1 Collocation FEM Method

In collocation method, δ is the Dirac delta function. Thus the weighted residual equation in the collocation method takes the form

$$\int_{\Omega} R(x,y,z)\delta(x-x_i)(y-y_i)(z-z_i)d\Omega \qquad (a)$$

using the property of the delta function, this equation (a) reduces to

$$R(x,y,z)\big]_{x_i,y_i,z_i} = 0 \qquad \text{for } i = 1,2......M$$

where M is the number of collocation points in an element.

Substituting the approximation of $\hat{u}(x,y,z)$ in R (x,y,z) we have

$$\Big[\sum_{i=1}^{k} U_i L(N_i(x,y,z)) - f\Big]_{x_i,y_i,z_i} = 0 \qquad \text{for } i = 1,2,3......M$$

$$\sum_{i=1}^{k} U_i L(N_i(x_i,y_i,z_i)) - f_i = 0 \qquad \text{for } i = 1,2,3......M$$

The evaluation of the above equation at M collocation points results with M algebraic equations. Solution of these M equations yields the unknown coefficients U_i defining U(x,y,z). In otherwords, U_i is the approximate numerical solution of the differential equation L(u) = f.

The collocation approach, when applied to a descritized mesh, provides the advantage of Finite Element method with following additional attractive features.

i) collocation methodology, applied in conjunction with finite elements, offers an approach that is

a) conceptually simple

b) mathematically straight forward and

c) preserves the fundamental advantages of the finite element method.

ii) collocation methods do not require integration procedures in the formulation of the approximating equations

iii) The resulting matrix equation exhibits a coefficient stucture that may be amenable to efficient solution using modern methods in matrix algebra.

An apparent disadvantage to collocation methods is the predisposition to use basis functions of higher continuity. The most commonly used member of this family of functions is the hermite cubic polynomials.

4.4.2 Number of Collocation Points

The number of collocation points to be used is very important. In fact the number of collocation points depend on the number of degrees of freedom for each node.

In problems with N_p nodes and K degrees of freedom per node, we have $N=(N_p)(K)$ total degrees of freedom. To solve M algebraic equations obtained from M collocation points, M should be such that it equals the total active degrees of freedom (i.e the total degrees of freedom excluding the boundary conditions). In a regular subspace, such as rectangles, Hermitian element having four degrees of freedom per node is dictated by the need to have the same number of unknowns as the equations.

4.5 COLLOCATION FINITE ELEMENT FORMULATIONS.

4.5.1 One-dimensional Groundwater Flow Equation

$$\frac{\partial}{\partial x}(K_x\frac{\partial h}{\partial x}) - S\frac{\partial h}{\partial t} - f = 0$$

$$K_x\frac{\partial^2 h}{\partial x^2} + \frac{\partial K_x}{\partial x}\frac{\partial h}{\partial x} - S\frac{\partial h}{\partial t} - f = 0$$

Using the following approximations,

$$\hat{K}_x = \sum_{i=1}^{Npe} N_{K_i} K_i$$

$$\hat{h} = \sum_{i=1}^{ND} N_j h_j$$

$$\hat{f} = \sum_{i=1}^{Npe} N_{fi} f_i$$

where, h_j = head at node 'i', when j is odd

$\frac{\partial h}{\partial x}$ = first derivative of head at node i, when j is even.

N_{K_i} = basis/shape function for the interpolation of K at node 'i'.

N_{fi} = basis/shape function for the interpolation of f at node i.

N_j = the shape function for h_j

N_{pe} = Number of nodes per element

N_D = Number of nodes per element times D.O.F per node.

Since $S = \rho g[\alpha(1-\eta)+\eta\beta]$, and α and β are very small in magnitude, S can be assumed to be independent of ρ and η.

Now substituting the above approximations into the governing equation and for M collocation points in the element , we obtain

$$[\sum_{i=1}^{Npc} N_{K_i} K_i \frac{\partial^2}{\partial x^2}(\sum_{j=1}^{ND} N_j h_j) + \frac{\partial}{\partial x}(\sum_{i=1}^{Npc} K_i N_{Ki}) \frac{\partial}{\partial x}(\sum_{j=1}^{ND} N_j h_j) - S\frac{\partial}{\partial t}(\sum_{j=1}^{ND} N_j h_j) - \sum_{i=1}^{Npc} N_{fi} f_i]_{x_l} = 0$$

$l = 1,2,3 \ldots\ldots M$

$$[\sum_{i=1}^{Npc} N_{K_i} K_i \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial x^2} h_j + \sum_{i=1}^{Npc} \frac{\partial N_{K_i}}{\partial x} K_i \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x} h_j - S\sum_{j=1}^{ND} N_j \frac{\partial h_j}{\partial t} - \sum_{i=1}^{Npc} N_{fi} f_i]_{x_l} = 0.$$

$l = 1,2,\ldots\ldots M.$

Writting the above in matrix notations, we have

$$\{[[A_1][A_2] + [B_1][B_2]]\{H\} - [C_1]\{\frac{\partial h}{\partial t}\} - \{F\}\}_{x_l} = 0$$

where

$$[A_1] = \sum_{i=1}^{Npc} N_{K_i} K_i$$

$$[A_2] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial x^2}$$

$$[B_1] = \sum_{i=1}^{Npc} \frac{\partial N_{K_i}}{\partial x} K_i$$

$$[B_2] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x}$$

$$[C_1] = S\sum_{j=1}^{ND} N_i$$

$$\{F\} = \sum_{i=1}^{Npe} N_{fi} f_i$$

$$\{H\} = [h_1\ h_2 \ldots\ldots h_{ND}]^T$$

$$\{\frac{\partial h}{\partial t}\} = [\frac{\partial h_1}{\partial t}\ \frac{\partial h_2}{\partial t} \ldots\ldots \frac{\partial h_{ND}}{\partial t}]^T$$

In global form, the matrix equation is

$$\{[G]\{H\} - [C]\{\frac{\partial h}{\partial t}\} = \{F\}\}_{x_1.}$$

where

$$[G] = [[A_1][A_2] + [B_1][B_2]]$$

4.5.2 One-dimensional Transport Equation

$$\frac{\partial}{\partial x}(D_x\frac{\partial C}{\partial x}) - \frac{\partial}{\partial x}(V_x C) - S_a C = \eta\frac{\partial C}{\partial t}$$

$$D_x\frac{\partial^2 C}{\partial x^2} + \frac{\partial D_x}{\partial x}\frac{\partial C}{\partial x} - C\frac{\partial V_x}{\partial x} - V_x\frac{\partial C}{\partial x} - S_a C = \eta\frac{\partial C}{\partial t}$$

Using the following approximations,

$$\hat{D}_x = \sum_{i=1}^{Npe} N_{D_i} D_i$$

$$\hat{V}_x = \sum_{i=1}^{Npe} N_{V_i} V_i$$

$$\hat{C} = \sum_{j=1}^{ND} N_j C_j$$

$$\hat{S}_a = \sum_{i=1}^{Npe} N_{Si} S_i$$

$$\hat{\eta} = \sum_{i=1}^{Npe} N_{\eta i} \eta_i$$

where, .

C_j = concentration at node 'i', when j is odd

$\frac{\partial C}{\partial x}$ = first derivative of concentration at node i, when j is even.

N_{D_i} = basis/shape function for the interpolation of D at node 'i'.

N_{V_i} = basis/shape function for the interpolation of V at node 'i'.

N_{Si} = basis/shape function for the interpolation of S_a at node i.

N_j = the shape function for C_j

N_{pe} = Number of nodes per element

N_D = Number of nodes per element times D.O.F per node.

Now substituting the above approximations into the governing equation and for M collocation points in the element , we obtain

$$[\sum_{i=1}^{Npc} N_{D_i} D_i \frac{\partial^2}{\partial x^2}(\sum_{j=1}^{ND} N_j C_j) + \frac{\partial}{\partial x}(\sum_{i=1}^{Npc} D_i N_{Di}) \frac{\partial}{\partial x}(\sum_{j=1}^{ND} N_j C_j) - \sum_{i=1}^{Npc} N_{Vi} V_i \frac{\partial}{\partial x}(\sum_{j=1}^{ND} N_j C_j)$$

$$- \sum_{j=1}^{ND} N_j C_j \frac{\partial}{\partial x}(\sum_{i=1}^{Npc} N_{Vi} V_i) - \sum_{i=1}^{Npc} N_{si} S_i \sum_{j=1}^{ND} N_j C_j = \sum_{i=1}^{Npc} N_{\eta i} \eta_i \frac{\partial}{\partial t}(\sum_{j=1}^{ND} N_j C_j)]_{x_l}$$

$l = 1,2,3 \ldots\ldots.. M$

$$[\sum_{i=1}^{Npc} N_{D_i} D_i \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial x^2} C_j + \sum_{i=1}^{Npc} \frac{\partial N_{D_i}}{\partial x} D_i \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x} C_j - \sum_{i=1}^{Npc} N_{Vi} V_i \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x} C_j - \sum_{i=1}^{Npc} \frac{\partial N_{Vi}}{\partial x} V_i \sum_{j=1}^{ND} N_j C_j -$$

$$\sum_{i=1}^{Npc} N_{Si} S_i \sum_{j=1}^{ND} N_j C_j = \sum_{i=1}^{Npc} N_{\eta i} \eta_i \sum_{j=1}^{ND} N_j \frac{\partial C_j}{\partial t}]_{x_l}$$

$l = 1,2, \ldots\ldots. M.$

Writting the above in matrix notations, we have

$$\{[[A_1][A_2] + [B_1][B_2] - [C_1][B_2] - [D_1][R_1] - [E_1][R_1]]\{C\} = [F_1][R_1]\{\frac{\partial C}{\partial t}\}\}_{x_l}$$

where $[A_1] = \sum_{i=1}^{Npc} N_{Di} D_i$

$$[A_2] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial x^2}$$

$$[B_1] = \sum_{i=1}^{Npc} \frac{\partial N_{Di}}{\partial x} D_i$$

$$[B_2] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x}$$

$$[C_1] = \sum_{i=1}^{Npe} N_{Vi} V_i$$

$$[D_1] = \sum_{i=1}^{Npe} \frac{\partial N_{Vi}}{\partial x} V_i$$

$$[E_1] = \sum_{i=1}^{Npe} N_{si} S_i$$

$$[F_1] = \sum_{i=1}^{Npe} N_{\eta i} \eta_i$$

$$[R_1] = \sum_{j=1}^{ND} N_j$$

$$\{C\} = [C_1\ C_2 \ldots\ldots C_{ND}]^T$$

$$\{\frac{\partial C}{\partial t}\} = [\frac{\partial C_1}{\partial t}\ \frac{\partial C_2}{\partial t} \ldots\ldots \frac{\partial C_{ND}}{\partial t}]^T$$

In global form, the matrix equation is

$$\{[G]\{C\} = [P]\{\frac{\partial C}{\partial t}\}\ \}_{x_1}$$

Where

$$[P] = [F_1][R_1]$$

$$[G] = [[A_1][A_2] + [B_1][B_2] - [C_1][B_2] - [D_1][R_1] - [E_1][R_1]]$$

4.5.3 Two-dimensional Groundwater Flow Equation

$$\frac{\partial}{\partial x}(K_x\frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(K_y\frac{\partial h}{\partial y}) = S\frac{\partial h}{\partial t} + f$$

Using the following approximations for the variables

$$\hat{K}_x = \sum_{i=1}^{Npe} N_{ki}K_{xi}$$

$$\hat{K}_y = \sum_{i=1}^{Npe} N_{ki}K_{yi}$$

$$\hat{h} = \sum_{j=1}^{ND} N_j h_j$$

$$\hat{f} = \sum_{i=1}^{Npe} N_{fi}f_i$$

Substituting the above approximations in the governing differential equation, we obtain for M collocation points

$$[\sum_{i=1}^{Npe}\frac{\partial N_{ki}}{\partial x}K_{xi}\sum_{j=1}^{ND}\frac{\partial N_j}{\partial x}h_j + \sum_{i=1}^{Npe}N_{ki}K_{xi}\sum_{j=1}^{ND}\frac{\partial^2 N_j}{\partial^2 x}h_j + \sum_{i=1}^{Npe}\frac{\partial N_{ki}}{\partial y}K_{yi}\sum_{j=1}^{ND}\frac{\partial N_j}{\partial y}h_j + \sum_{i=1}^{Npe}N_{ki}K_{yi}\sum_{j=1}^{ND}\frac{\partial^2 N_j}{\partial^2 y}h_j$$

$$= S\sum_{j=1}^{ND}N_j\frac{\partial h_j}{\partial t} + \sum_{i=1}^{Npe}N_{fi}f_i]_{x_l,y_l}$$

where l = 1,2......M , M is the number of collocation points to be used per element.

Writing in matrix notations, we obtain

$$\{[[A_x][B_x] + [C_x][D_x] + [A_y][B_y] + [C_y][D_y]]\{H\} = [A_T]\{\frac{\partial h}{\partial t}\} + \{F\}\}_{x_l,y_l}$$

Where

$$[A_x] = \sum_{i=1}^{Npc} \frac{\partial N_{ki}}{\partial x} K_{xi}$$

$$[B_x] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x}$$

$$[C_x] = \sum_{i=1}^{Npc} N_{ki} K_{xi}$$

$$[D_x] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial^2 x}$$

$$[A_y] = \sum_{i=1}^{Npc} \frac{\partial N_{ki}}{\partial y} K_{yi}$$

$$[B_y] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial y}$$

$$[C_y] = \sum_{i=1}^{Npc} N_{ki} K_{yi}$$

$$[D_y] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial^2 y}$$

$$[A_T] = S \sum_{j=1}^{ND} N_j$$

$$\{F\} = \sum_{i=1}^{Npc} N_{fi} f_i$$

All these matrices are evaluated at the collocation points in each element. The final global matrix form, obtained after assembling the element matrices, can be written as

$$\{[G]\{H\} = [P]\{\frac{\partial h}{\partial t}\} + \{F\}\}_M$$

where

$$[G] = [[A_x][B_x] + [C_x][D_x] + [A_y][B_y] + [C_y][D_y]]_{x_i,y_i}$$

4.5.4 Two-dimensional Transport Equation

$$\frac{\partial}{\partial x}(D_x\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_y\frac{\partial C}{\partial y}) - V_x\frac{\partial C}{\partial x} - C\frac{\partial V_x}{\partial x} - V_y\frac{\partial C}{\partial y} - C\frac{\partial V_y}{\partial y} - S_aC = \eta\frac{\partial C}{\partial t}$$

Using the following approximations for the variables

$$\hat{D}_x = \sum_{i=1}^{Npe} N_{Di}D_{xi}$$

$$\hat{D}_y = \sum_{i=1}^{Npe} N_{Di}D_{yi}$$

$$\hat{V}_x = \sum_{i=1}^{Npe} N_{Vi}V_{xi}$$

$$\hat{V}_y = \sum_{i=1}^{Npe} N_{Vi}V_{yi}$$

$$\hat{C} = \sum_{j=1}^{ND} N_jC_j$$

$$\hat{S}_a = \sum_{i=1}^{Npe} N_{si}S_{si}$$

$$\hat{\eta} = \sum_{i=1}^{Npe} N_{\eta i}\eta_i$$

Substituting the above approximations in the governing differential equation, we obtain for M collocation points

$$[\sum_{i=1}^{Npe}\frac{\partial N_{Di}}{\partial x}D_{xi}\sum_{j=1}^{ND}\frac{\partial N_j}{\partial x}C_j + \sum_{i=1}^{Npe}N_{Di}D_{xi}\sum_{j=1}^{ND}\frac{\partial^2 N_j}{\partial^2 x}C_j + \sum_{i=1}^{Npe}\frac{\partial N_{Di}}{\partial y}D_{yi}\sum_{j=1}^{ND}\frac{\partial N_j}{\partial y}C_j + \sum_{i=1}^{Npe}N_{Di}D_{yi}\sum_{j=1}^{ND}\frac{\partial^2 N_j}{\partial^2 y}C_j -$$

$$\sum_{i=1}^{Npc} N_{Vi} V_{xi} \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x} C_j - \sum_{i=1}^{Npc} \frac{\partial N_{Vi}}{\partial y} V_{xi} \sum_{j=1}^{ND} N_j C_j - \sum_{i=1}^{Npc} N_{Vi} V_{yi} \sum_{j=1}^{ND} \frac{\partial N_j}{\partial y} C_j - \sum_{i=1}^{Npc} \frac{\partial N_{Vi}}{\partial y} V_{yi} \sum_{j=1}^{ND} N_j C_j$$

$$- \sum_{i=1}^{Npc} N_{Si} S_i \sum_{j=1}^{ND} N_j C_j = \sum_{i=1}^{Npc} N_{\eta i} \eta_i \sum_{j=1}^{ND} N_j \frac{\partial C_j}{\partial t} \,]_{x_l, y_l}$$

where $l = 1,2......M$, M is the number of collocation points to be used per element.

Writing in matrix notations, we obtain

$$\{[[A_x][B_x] + [C_x][D_x] + [A_y][B_y] + [C_y][D_y] - [E_x][B_x] - [E_y][B_y] - [F_x][A_T] -$$

$$[F_y][A_T] - [S][A_T]]\{C\} = [H][A_T]\{\frac{\partial h}{\partial t}\}\}_{x_l, y_l}$$

Where

$$[A_x] = \sum_{i=1}^{Npc} \frac{\partial N_{Di}}{\partial x} D_{xi}$$

$$[B_x] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial x}$$

$$[C_x] = \sum_{i=1}^{Npc} N_{Di} D_{xi}$$

$$[D_x] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial^2 x}$$

$$[E_x] = \sum_{i=1}^{Npc} N_{Vi} V_{xi}$$

$$[F_x] = \sum_{i=1}^{Npc} \frac{\partial N_{Vi}}{\partial x} V_{xi}$$

$$[A_y] = \sum_{i=1}^{Npe} \frac{\partial N_{Di}}{\partial y} D_{yi}$$

$$[B_y] = \sum_{j=1}^{ND} \frac{\partial N_j}{\partial y}$$

$$[C_y] = \sum_{i=1}^{Npe} N_{Di} D_{yi}$$

$$[D_y] = \sum_{j=1}^{ND} \frac{\partial^2 N_j}{\partial^2 y}$$

$$[E_y] = \sum_{i=1}^{Npe} N_{Vi} V_{yi}$$

$$[F_y] = \sum_{i=1}^{Npe} \frac{\partial N_{Vi}}{\partial y} V_{yi}$$

$$[H] = \sum_{i=1}^{Npe} N_{\eta i} \eta_i$$

$$[A_T] = \sum_{j=1}^{ND} N_j$$

$$[S] = \sum_{i=1}^{Npe} N_{Si} S_i$$

All these matrices are evaluated at the collocation points in each element. The final global matrix form, obtained after assembling the element matrices, can be written as

$$\{[G]\{C\} = [P]\{\frac{\partial C}{\partial t}\}\}_M \tag{A}$$

where

$$[\{P] = [H]\,[A_T]$$

$$[G] = [[A_x][B_x] + [C_x][D_x] + [A_y][B_y] + [C_y][D_y] - [E_x][B_x] - [E_y][B_y] - [F_x][A_T] - [F_y][A_T] - [S][A_T]\,]_{x_i, y_i}$$

4.6 TIME STEPPING SCHEME

Since the D.O.F $\hat{C}_j$ and the matrices [G] and [P] (for the transport equation) and the vector {F} are time dependent, they can be approximated by a weighted average of their values before and after the small time interval Δt. The time derivative $\frac{\partial \hat{C}_i}{\partial t}$ may be approximated by the forward finite difference scheme as

$$\frac{\partial \hat{C}_j}{\partial t} = \frac{\hat{C}_{j_{t+\Delta t}} - \hat{C}_{j_t}}{\Delta t} \qquad (1)$$

and

$$\hat{C}_j = \theta_c \hat{C}_{j_{t+\Delta t}} + (1-\theta_c)\hat{C}_{j_t} \qquad (2)$$

$$[G] = \theta_M [G]_{t+\Delta t} + (1-\theta_M)[G]_t \qquad (3)$$

$$[P] = \theta_M [P]_{t+\Delta t} + (1-\theta_M)[P]_t \qquad (4)$$

$$\{F\} = \theta_M \{F\}_{t+\Delta t} + (1-\theta_M)\{F\}_t \qquad (5)$$

where

$0 \le \theta_c \le 1 \rightarrow$ the degree of implicitness for $\hat{C}_j$ and $0 \le \theta_M \le 1 \rightarrow$ the degree of implicitness for the matrices and vectors

Substituting (1)-(5) into the FEM equations

$$\{\theta_M [G]_{t+\Delta t} + (1-\theta_M)[G]_t\}[\theta_c \{C\}_{t+\Delta t} + (1-\theta_c)\{C\}_t] -$$

$$[\, \theta_M [P]_{t+\Delta t} + (1-\theta_M)[P]_t][\frac{\{C\}_{t+\Delta t} - \{C\}_t}{\Delta t}] = 0$$

$$[L]\{C\}_{t+\Delta t} = [M]\{C\}_t$$

where

$$[L] = \theta_c\{\theta_M[G]_{t+\Delta t} + (1-\theta_M)[G]_t\} - \frac{1}{\Delta t}[\,\theta_M[P]_{t+\Delta t} + (1-\theta_M)[P]_t]$$

$$[M] = -\,[(1-\theta_c)\{\theta_M[G]_{t+\Delta t} + (1-\theta_M)[G]_t\} + \frac{1}{\Delta t}[\,\theta_M[P]_{t+\Delta t} + (1-\theta_M)[P]_t]]$$

if $\theta_M = 0$, i.e. the coefficient Matrices are assumed to be invariant in time, then

$$[L] = \theta_c[G] - \frac{1}{\Delta t}[P]$$

$$[M] = -\,(1-\theta_c)[G] - \frac{1}{\Delta t}[P]$$

4.7 BASIS FUNCTIONS

4.7.1 Cubic Hermitian Bases in One-dimension

The typical finite element formulation involves the definition of the basis function in a local coordinate system, and then formulation of the collocation equations on an element by element basis.

For the development of one-dimensional cubic Hermitian bases for two noded elements, a third order polynomial in ξ is assumed. The four unknown coefficients are determined by prescribing the values of the dependent variable and its derivative at each of the two nodes. These Cubic Hermitian basis functions guarantee the continuity of the dependent variable and its first derivatives and hence are C^1 – continuous. The four basis functions can be written as

$$ {}^{3}H_1^0(\xi) = \frac{1}{4}(\xi-1)^2(\xi+2) $$

$$ {}^{3}H_1^1(\xi) = \frac{1}{4}(\xi-1)^2(\xi+1) $$

$$ {}^{3}H_2^0(\xi) = \frac{1}{4}(\xi+1)^2(-\xi+2) $$

$$ {}^{3}H_2^1(\xi) = \frac{1}{4}(\xi+1)^2(\xi-1) $$

for $-1 \le \xi \le 1$

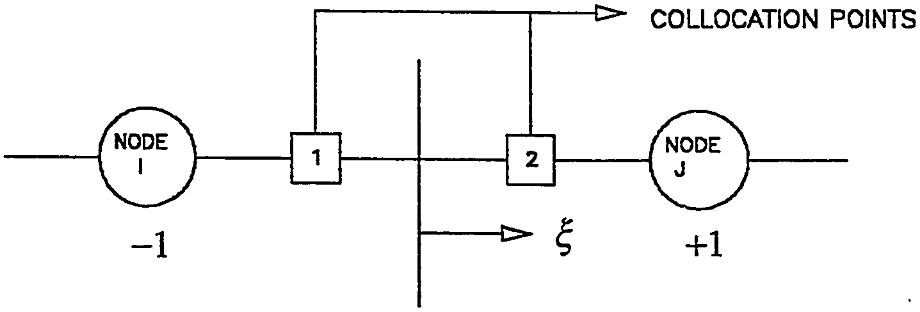


Figure-4.2 : One-dimensional 2-noded element with two collocation points

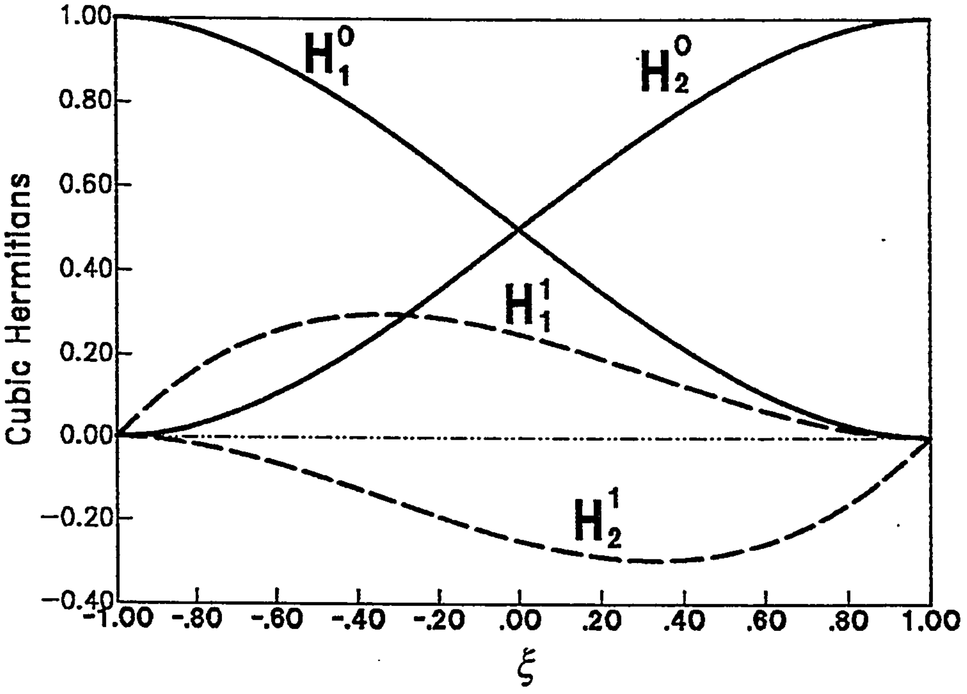


Figure-4.3 : One-dimensional Cubic Hermitian Basis Functions

where

${}^{L}H_k^{n}(\xi)$,

L -- degrees of Hermitian Polynomial,

n -- indicates the order of degrees of freedom, and

k -- the node numbers.

A typical one-dimensional 2-noded element with two collocation points and the corresponding cubic hermitians are shown in figure-4.2 and figure-4.3 respectively.

4.7.2 Relationship Between the Local and Global Coordinate System

In local coordinate system, $\hat{C}^e$ is approximated over a cubic Hermitian element as

$$\hat{C}^e(\xi) = \sum_{k=1}^{2}[C_k{}^3H_k{}^o(\xi) + {\frac{dc_k}{d\xi}}^{3} H_k{}^1(\xi)] \qquad (1)$$

And in terms of global coordinate system, we have

$$\hat{C}^e(x) = \sum_{k=1}^{2}[C_k{}^3H_k{}^o(x) + {\frac{dc_k}{dx}}^{3} H_k{}^1(x) \qquad (2)$$

To evaluate the relationship between $\hat{C}^e(\xi)$ and $\hat{C}^e(x)$ under a given coordinate transformation system (C_T) which expresses x in term of ξ i.e,x = f(ξ), it is necessary to transform each element via a linear relationship between x and ξ. For unequal element lengths this linear C_T yields a C^0 – continuity only.

The linear C_T defined over an element and using local node numbering can be written as

$$x(\xi) = \frac{x_2 + x_1}{2} + \frac{x_2 - x_1}{2}\xi$$

$$\text{or } \xi(x) = \frac{2}{x_2 - x_1}(x - \frac{x_2 + x_1}{2})$$

$$= \frac{2}{\Delta L^e}(x - \frac{x_2 + x_1}{2}) \quad \text{where } \Delta L^e = x_2 - x_1$$

From $x(\xi)$, we have

$$\frac{dx}{d\xi} = \frac{\Delta L^e}{2}$$

The general form of the piecewise Cubic Hermitian polynomials in global coordinate system can be written as follows

$$^3H_k^0(x) = \frac{(x-x_{k-1})^2}{(x_k - x_{k-1})^3}[2(x_k - x) + (x_k - x_{k-1})] \quad x_{k-1} \le x \le x_k$$

$$= \frac{(x_{k+1}-x)^2}{(x_{k+1}-x_{k)}^3}[3(x_{k+1} - x_k)-2(x_{k+1}-x)] \quad x_k \le x \le x_{k+1}$$

$$= 0 \text{ Elsewhere.}$$

$$^3H_k^1(x) = \frac{(x-x_{k-1})^2(x - x_{k)}}{(x_k - x_{k-1})^2} \quad x_{k-1} \le x \le x_k$$

$$= \frac{(x_{k+1}-x)^2(x - x_k)}{(x_{k+1}-x_k)^2} \quad x_k \le x \le x_{k+1}$$

$= 0$ Elsewhere.

For an element, which reduces to ,

$$.{}^3H_1^0(x) = \frac{(x-x_0)^2}{(x_1-x_0)^3}[2(x_1-x)+(x_1-x_0)]$$

Substituting $x=f(\xi)$ in the above equation, we can easily prove that

$$.{}^3H^0{}_2(x) = .{}^3H^0{}_2(\xi)$$

Similarly , it can be shown that ,

$$.{}^3H^0{}_1(x) = .{}^3H^0{}_1(\xi)$$

$$.{}^3H^1{}_1(x) = .{}^3H^1{}_1(\xi)\frac{\Delta L^e}{2}$$

$$.{}^3H^1{}_2(x) = .{}^3H^1{}_2(\xi)\frac{\Delta L^e}{2}$$

Now,

$$\hat{C}^e(\xi) = \sum_{k=1}^{2}(C_K\,{}^3H^0{}_k(\xi) + \frac{dC_k}{d\xi}\,{}^3H^1{}_k(\xi))$$

or

$$\hat{C}^e(\xi) = \sum_{k=1}^{2}(C_K\,{}^3H^0{}_k(\xi) + \frac{dC_k}{dx}.\frac{dx}{d\xi}\,{}^3H^1{}_k(\xi))$$

or

$$\hat{C}^e(\xi) = \sum_{k=1}^{2}(C_K\,{}^3H^0{}_k(\xi) + \frac{dC_k}{dx}.\frac{\Delta L^e}{2}\,{}^3H^1{}_k(\xi))$$

or

$$\hat{C}^e(\xi) = \sum_{k=1}^{2}(C_K\, {}^3H^0_k(x) + \frac{dC_k}{dx}\, {}^3H^1_k(x))$$

or

$$\hat{C}^e(\xi) = \hat{C}^e(x)$$

Therefore $\hat{C}^e(\xi) = \hat{C}^e(x)$ requires a necessary condition that

$$N_{2k-1} = {}^3H^0_k(x) = {}^3H^0_k(\xi)$$

and

$$N_{2k} = {}^3H^1_k(x) = {}^3H^1_k(\xi).\frac{\Delta L^c}{2}$$

4.7.3 Cubic Hermitian Basis functions in Two-dimensions

C^1 - continuous two-dimensional cubic element has four degrees of freedom per node i.e. $C, \frac{\partial C}{\partial x}, \frac{\partial C}{\partial y}, \frac{\partial^2 C}{\partial x \partial y}$. Two-dimensional quadrilateral elements with 4 nodes has a total of (4X4) 16 degrees of freedom and requires 16 shape functions (e.g. N_i, i = 1,2......16). These shape functions, which involves two space variables, may be evaluated by the product of the one-dimensional Hermitians written in x and y seperately.

The form of approximate variable $\hat{C}$ over such an element can be written as

$$\hat{C} = \sum_{k=1}^{4}[C_k\, {}^{33}H_k^{00}(x,y) + \frac{\partial C_k}{\partial x}\, {}^{33}H_k^{10}(x,y) + \frac{\partial C_k}{\partial y}\, {}^{33}H_k^{01}(x,y) + \frac{\partial^2 C_k}{\partial x \partial y}\, {}^{33}H_k^{11}(x,y)\,]$$

where the summation is over the 4 nodes of the element.

.${}^{33}H_k^{nm}(x,y)$ - the two-dimensional Cubic Hermitian basis functions along the x and y directions and

n,m = 0, 1 indicates the order of degrees of freedom.

The more generalized two-dimensional form of $\hat{C}$, which is easier to code in computer, can be wrirren as a unified N_j

$$\hat{C} = \sum_{j=1}^{16} C_j N_j \quad j=1,2\,........16$$

where C_j represents sixteen degrees of freedom for an element, four per node ($\frac{\partial C}{\partial x}, \frac{\partial C}{\partial y}, \frac{\partial^2 C}{\partial x \partial y}$).

Using the one-dimensional basis functions, we have the following two-dimensional basis functions in ξ and ζ coordinate system:

$$N_1 = {}^3H_1^0(\xi).{}^3H_1^0(\zeta)$$
$$N_2 = {}^3H_1^1(\xi).{}^3H_1^0(\zeta)$$
$$N_3 = {}^3H_1^0(\xi).{}^3H_1^1(\zeta)$$
$$N_4 = {}^3H_1^1(\xi).{}^3H_1^1(\zeta)$$
$$N_5 = {}^3H_2^0(\xi).{}^3H_1^0(\zeta)$$
$$N_6 = {}^3H_2^1(\xi).{}^3H_1^0(\zeta)$$
$$N_7 = {}^3H_2^0(\xi).{}^3H_1^1(\zeta)$$
$$N_8 = {}^3H_2^1(\xi).{}^3H_1^1(\zeta)$$
$$N_9 = {}^3H_2^0(\xi).{}^3H_2^0(\zeta)$$
$$N_{10} = {}^3H_2^1(\xi).{}^3H_2^0(\zeta)$$
$$N_{11} = {}^3H_2^0(\xi).{}^3H_2^1(\zeta)$$
$$N_{12} = {}^3H_2^1(\xi).{}^3H_2^1(\zeta)$$
$$N_{13} = {}^3H_1^0(\xi).{}^3H_2^0(\zeta)$$
$$N_{14} = {}^3H_1^1(\xi).{}^3H_2^0(\zeta)$$
$$N_{15} = {}^3H_1^0(\xi).{}^3H_2^1(\zeta)$$
$$N_{16} = {}^3H_1^1(\xi).{}^3H_2^1(\zeta)$$

For $-1 \leq \xi \leq +1$ and $-1 \leq \zeta \leq +1$

And

$$C_{(4i-3)} = C_i$$

$$C_{(4i-2)} = (\frac{\partial C}{\partial x})_i$$

$$C_{(4i-1)} = (\frac{\partial C}{\partial y})_i$$

$$C_{4i} = (\frac{\partial^2 C}{\partial y \partial x})_i$$

A typical two-dimensional 4-noded element with 4 collocation points and the basis function, N_5 are shown in figure-4.4 and figure-4.5 respectively.

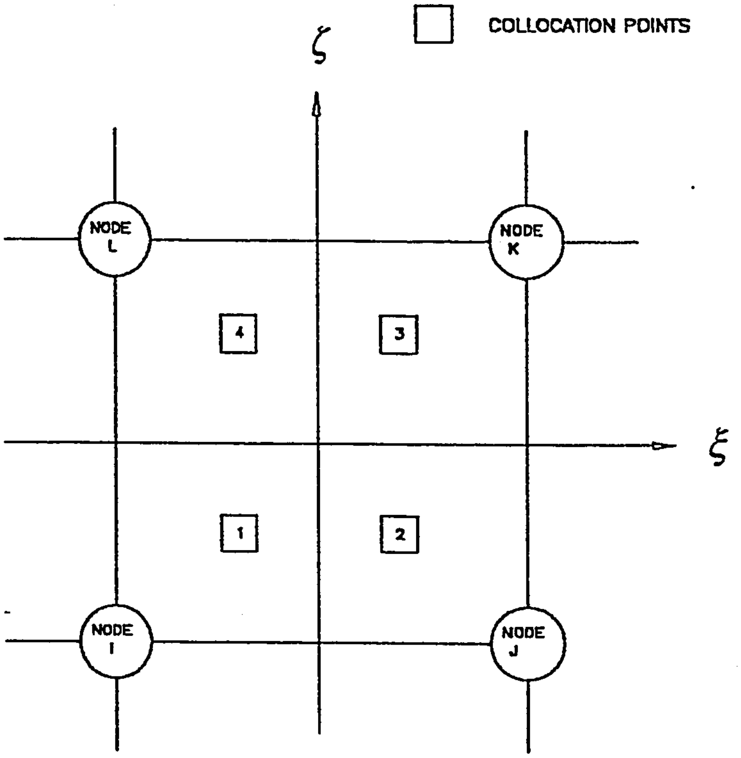


Figure-4.4 : Two-dimensional-4-noded elements with four collocation points

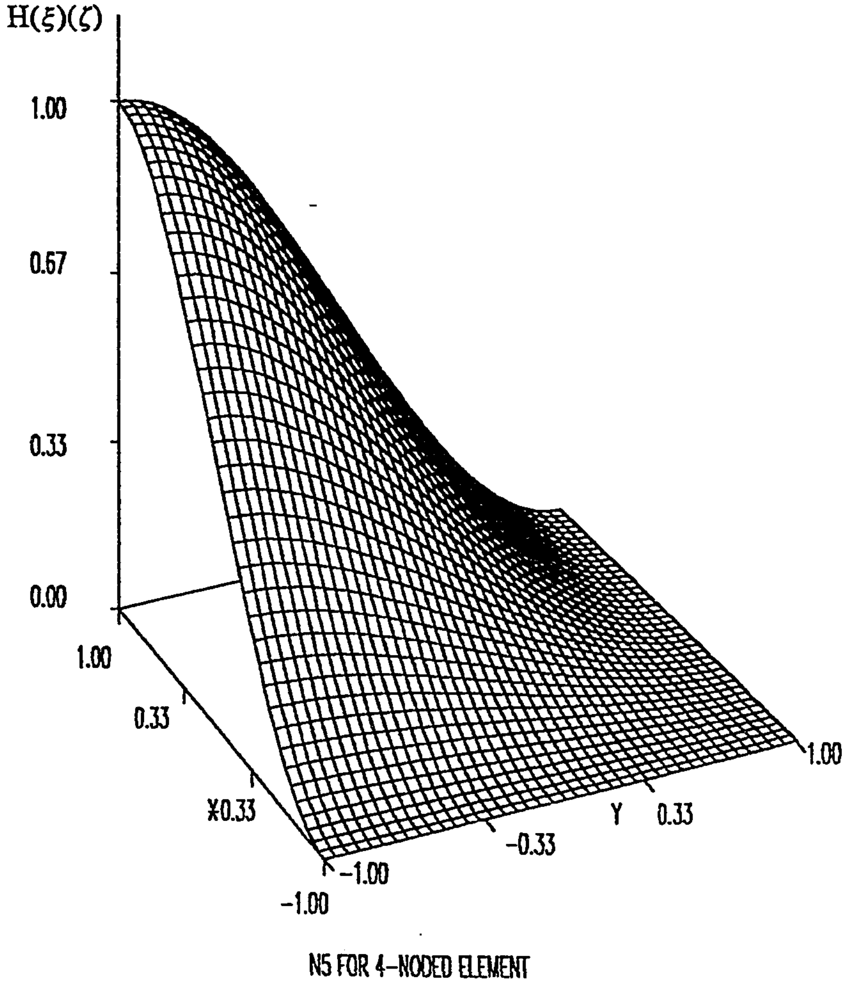


Figure-4.5 : Two-dimensional Hermitian Basis functions derived from one-dimensional cubic hermitians (figure-4.3)

4.8 SOLUTION ALGORITHM

In solving the coupled equations of groundwater flow and solute transport, the nature of the non-linearity should be considered. In these equations (Appendix-B1), the coefficients are non-linear functions of unknown variables. An iterative solution scheme is therefore indicated.

4.8.1 Steps in Iterative Scheme

1. The iterative routine starts at a given time step with an estimate of concentration distribution based on previous time step (i.e. initial values at the begining)

2. Evaluation of the concentration-dependent parameters in the groundwater flow equation for the estimated concentration distribution

3. Solution of the groundwater flow equation for the nodal values of head at the next time level

4. Computation of the nodal values of velocity, hydraulic conductivity, porosity, dispersion coefficient and the solute aggressiveness coefficient according to the appropriate additional equations and the updated values of head gradient

5. Solution of the transport equation using the updated parameters obtained in step-4 to predict the new concentration distribution

6.The procedure (step-3 to step-5) is repeated by evaluating the concentration-dependent parameters again with the updated values of concentration distribution and solving the governing equations at the same time level

7. The cycle is repeated untill the convergence criteria is satisfied

The repeatative solution of the system constitutes the dominant computational work in the overall algorithm. A Flow-Chart of this iterative scheme is shown in figure-4.6.

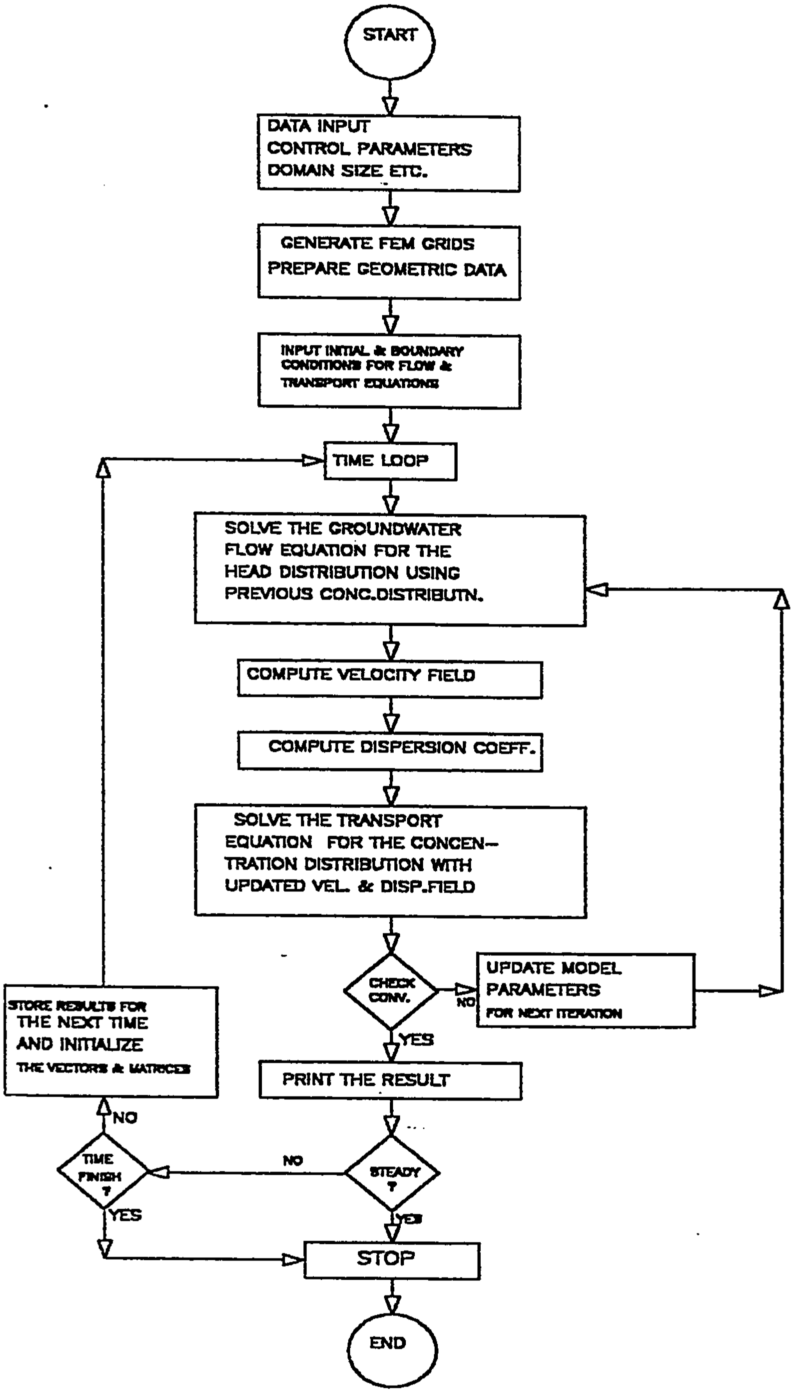


Figure-4.6 : Flow chart for the solution algorithm

CHAPTER V

NUMERICAL RESULTS AND DISCUSSIONS

Chapter V

NUMERICAL RESULTS AND DISCUSSIONS

5.1 INTRODUCTION

Computer programs are developed to solve the proposed system of equations. The Codes have the provision to solve the governing equations for a variety of combinations, namely

i) Groundwater flow equation only
ii) Transport Equation only
iii) Both equations for
    a) Non-coupled system
    b) Coupled system
        1. Non-Aggressive Solutes
        2. Aggressive Solutes

The Collocation Finite Element Method is used. A number of simple problems (figure-5.1) are solved to verify the accuracy of the numerical model. A brief discussions on different test problems are given below.

5.2 VERIFICATION OF THE MODEL WITH ANALYTICAL SOLUTIONS

The predictions of the developed model was compared with a number of problems having analytical solutions. Test run was also made for two simple problems previously solved by Smith (1985) using finite difference schemes. Both the one-dimensional and the two-dimensional programmes solved the problems with increased accuracy, supporting its superiority to finite difference methods.

Once the numerical model was tested, the following runs were made to study the applicability of the model.

a) Test Problem on Groundwater Flow

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) = S\frac{\partial h}{\partial t} + f \qquad 0 < x < L \qquad (5.1)$$

With

Initial Condition

$$h(x,0) = H(x)$$

Boundary Condition

$$h(0,t) = H_0 \text{ or } H_0(t) \quad \text{for} \quad 0 < t < t_0$$

$$h(L,t) = H_L$$

b) Test Problem on Solute Transport

$$\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(V_x C) - fC = \eta\frac{\partial C}{\partial t} \qquad 0 < x < L \qquad (5.2)$$

With

Initial Condition

$$C(x,0) = C(x)$$

Boundary Condition

$$C(0,t) = C_0 \text{ or } C_0(t) \quad \text{for } 0 < t < t_0$$

$$C(L,t) = C_L$$

Case A1 : Analytical solution for steady groundwater flow equation with constant K and f

$$h(x) = \frac{fx^2}{2K} + \{\frac{H_L - H_0}{L} - \frac{fL}{2K}\}x + H_0 \tag{5.3}$$

$$\frac{dh}{dx} = \frac{fx}{K} + \{\frac{H_L - H_0}{L} - \frac{fL}{2K}\} \tag{5.4}$$

Case A2 : Analytical solution for steady groundwater flow equation with $K = f = f(x) = \frac{1}{1+x}$ i.e. heterogeneous medium.

$$h(x) = \frac{(1+x)^2}{4}(2\ln(1+x) - 1) + C_1(x + \frac{x^2}{2}) + H_0 + \frac{1}{4} \tag{5.5}$$

$$\frac{dh}{dx} = (1+x)\ln(1+x) + C_1(1+x) \tag{5.6}$$

$$C_1 = \frac{\{H_L - H_0 - \frac{1}{4} - \frac{(1+L)^2}{4}(2\ln(1+L) - 1)\}}{(L + \frac{L^2}{2})}$$

Case B1 : Analytical solution for steady Solute Transport equation with constant D, V and f, and $C(0)=1$ and $C(1)=0$,

$$C(x) = a_1 e^{m_1 x} + a_2 e^{m_2 x} \tag{5.7}$$

$$\frac{dC}{dx} = a_1 m_1 e^{m_1 x} + a_2 m_2 e^{m_2 x} \tag{5.8}$$

$$m_1 = \frac{V}{2D} + \frac{1}{2D}\sqrt{V^2+4fD}$$

$$m_2 = \frac{V}{2D} - \frac{1}{2D}\sqrt{V^2+4fD}$$

$$a_1 = \frac{e^{m_2}}{e^{m_2} - e^{m_1}}$$

$$a_2 = \frac{e^{m_1}}{e^{m_1} - e^{m_2}}$$

Case B2 : Analytical solution for steady Solute Transport equation with D, V and f as function of x i.e. heterogeneous medium.

Defining $D = V = \frac{1}{1+x}$ and $f = \frac{4+2x}{(1+x)^2}$, we have ,

$$C(x) = b_1 e^{2x}(\frac{3x+2}{9}) + b_2 e^{-x} \tag{5.9}$$

$$\frac{dC}{dx} = b_1[(e^{2x}(\frac{3}{9}) + e^{2x}(\frac{2(3x+2)}{9})] - b_2 e^{-x} \tag{5.10}$$

$$b_1 = \frac{9}{[2 - e^{3L}(3L+2)]}$$

$$b_2 = 1 - \frac{2}{[2 - e^{3L}(3L+2)]}$$

The effects of $\frac{K}{f}$ ratio on head distribution is shown in figure-5.2. Figure-5.3 shows the solute movement patterns for different Peclet numbers $(\frac{VL}{D})$.

The developed model was found to be capable of producing satisfactory results compared to the analytical solutions (figure-5.4 and figure-5.5)

The solution of the unsteady groundwater flow and the transport equations also converged to the steady analytical solutions for both homogeneous and heterogeneous medium (figure-5.4c, figure-5.4d, figure-5.5c and figure-5.5d).

The two-dimensional model was verified with a variety of one-dimensional problems on two-dimensional space (Mohsen (1987), Bhuiyan et.al (1990)) and was found capable of producing satisfactory results.

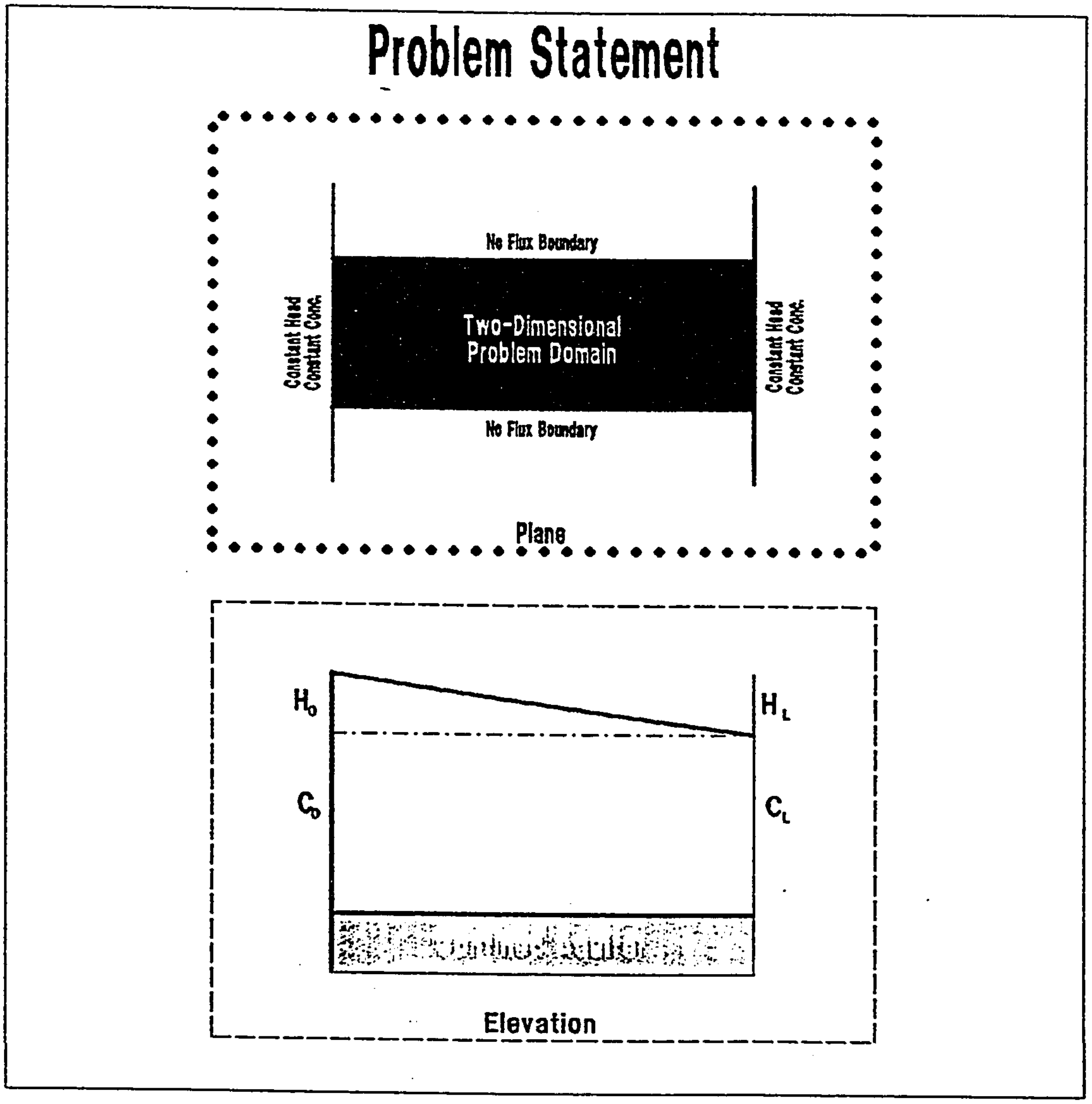


Figure-5.1: Problem statement in one-dimensional Analysis

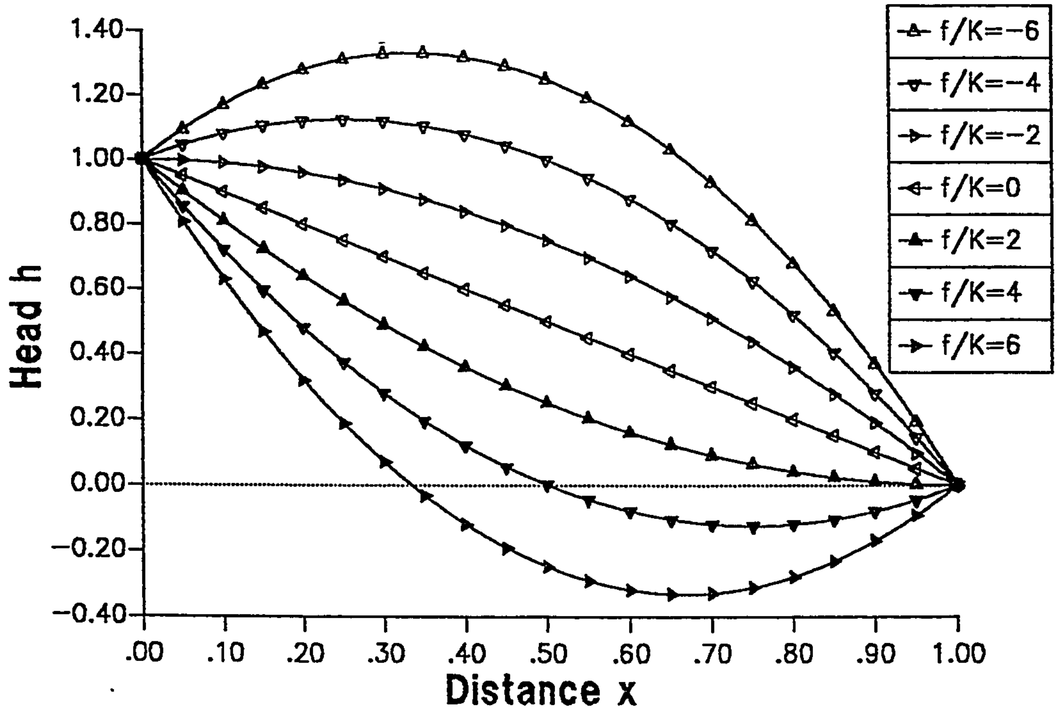


Figure-5.2: Effect of (f/K) ratio on Head Distribution (Equation 5.3)

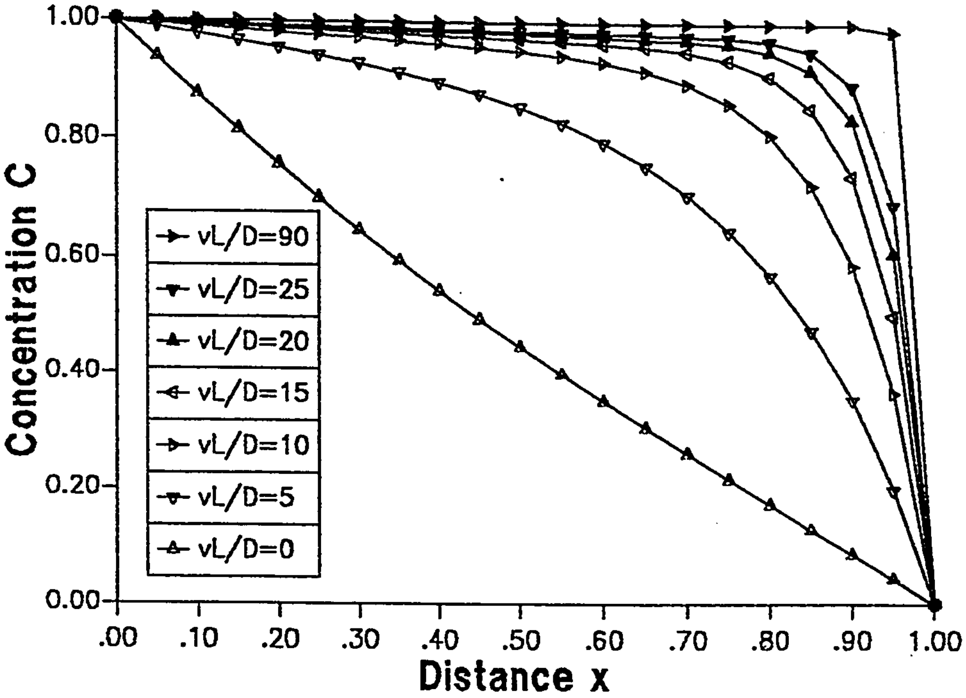


Figure-5.3: Effect of (VL/D) ratio on Concentration Distribution (Equation 5.7)

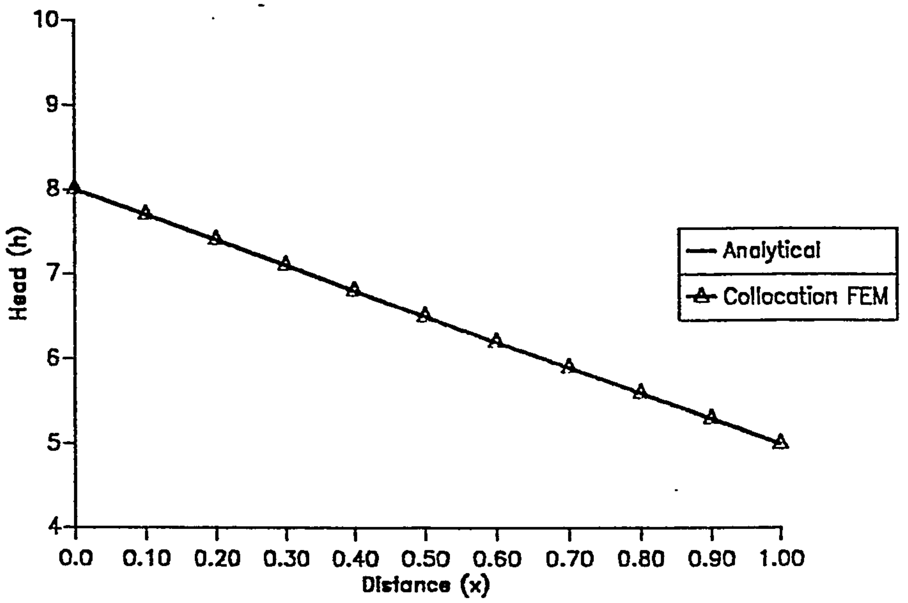


Figure-5.4a: Comparison of numerical and analytical solutions for steady groundwater flow equation (5.1) for homogeneous medium (constant K and f=0.0)

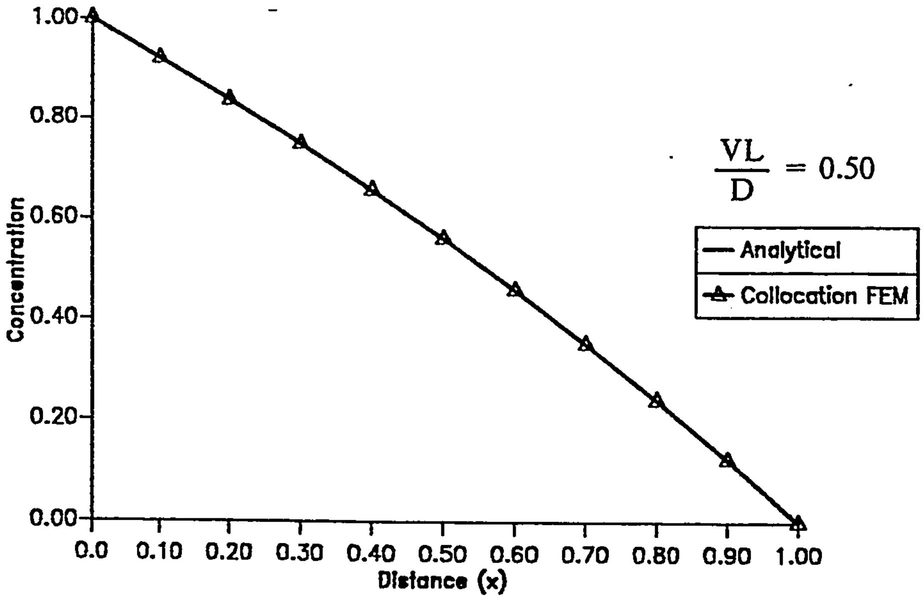


Figure-5.4b: Comparison of numerical and analytical solutions for steady solute transport equation (5.2) for homogeneous medium (constant D and V, and f=0.0)

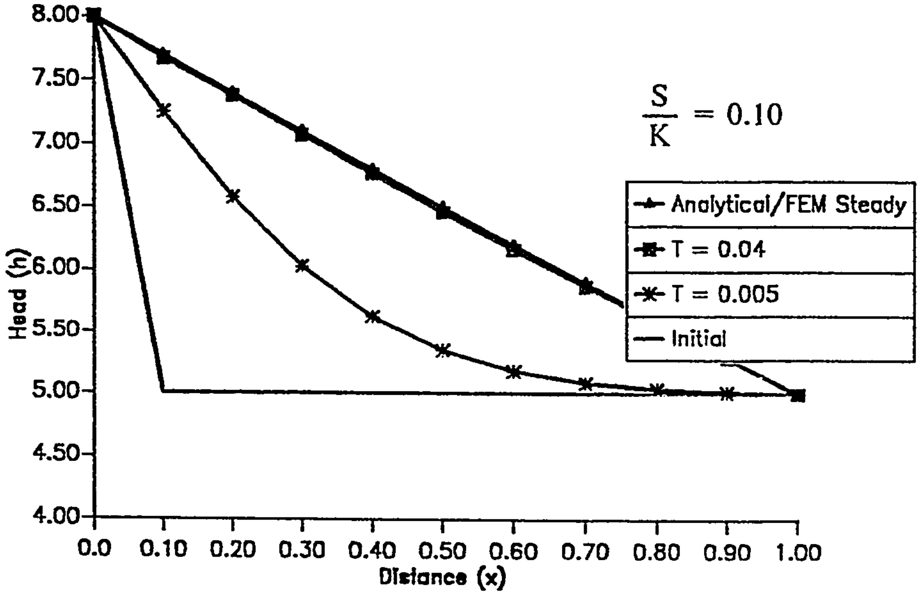


Figure-5.4c: Numerical solution of transient groundwater flow equation (5.1) for homogeneous medium (constant K and f=0.0)

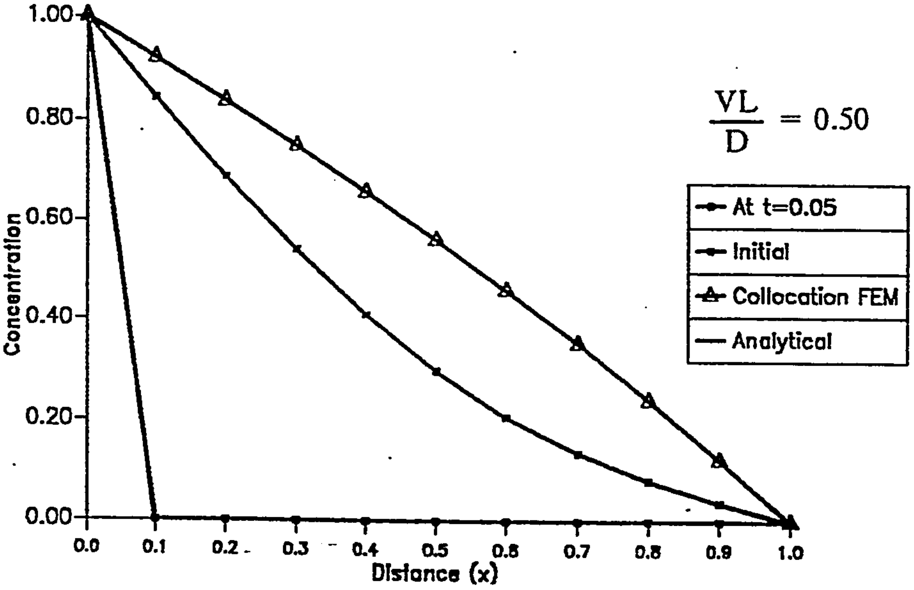


Figure-5.4d: Numerical solution of transient solute transport equation (5.2) for homogeneous medium (constant D and V, and f=0.0)

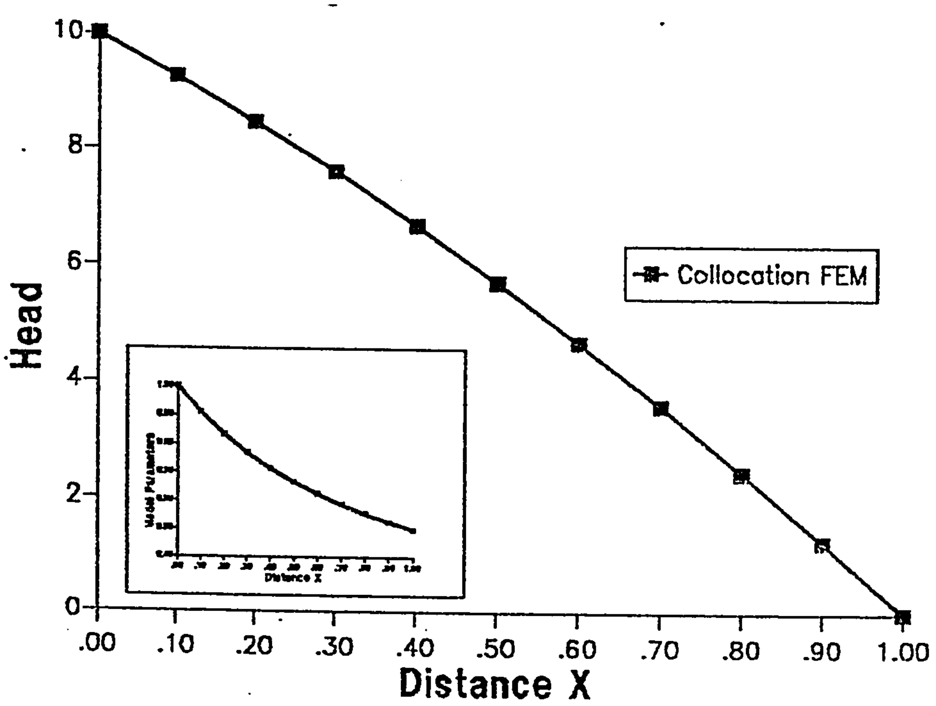


Figure-5.5a: Comparison of numerical and analytical solutions for steady groundwater flow equation (5.1) for heterogeneous medium ($K^{*} = \bar{f} = \frac{1}{1+x}$).

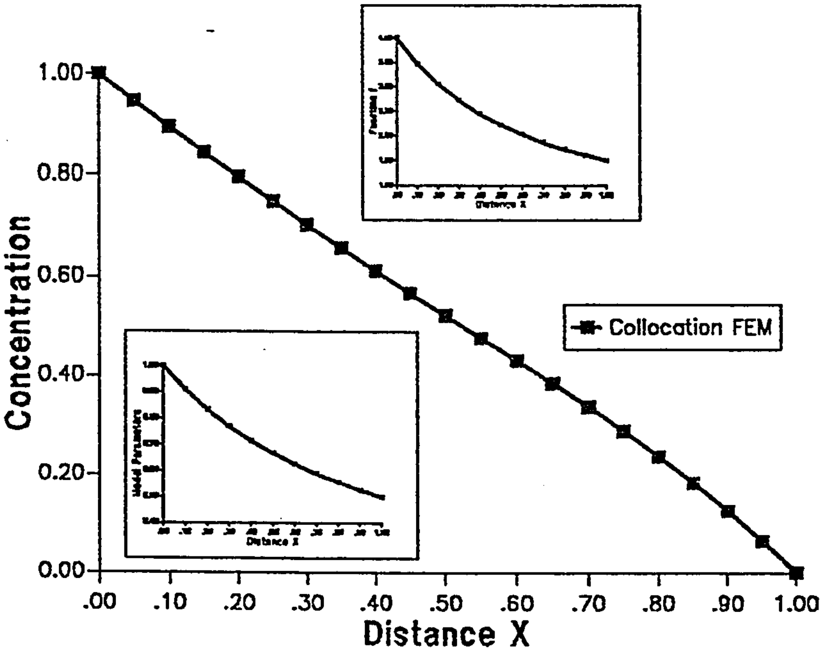


Figure-5.5b: Comparison of numerical and analytical solutions for steady solute transport equation (5.2) for heterogeneous medium ($D = V = \frac{1}{1+x}$ and $f = \frac{4+2x}{(1+x)^2}$)

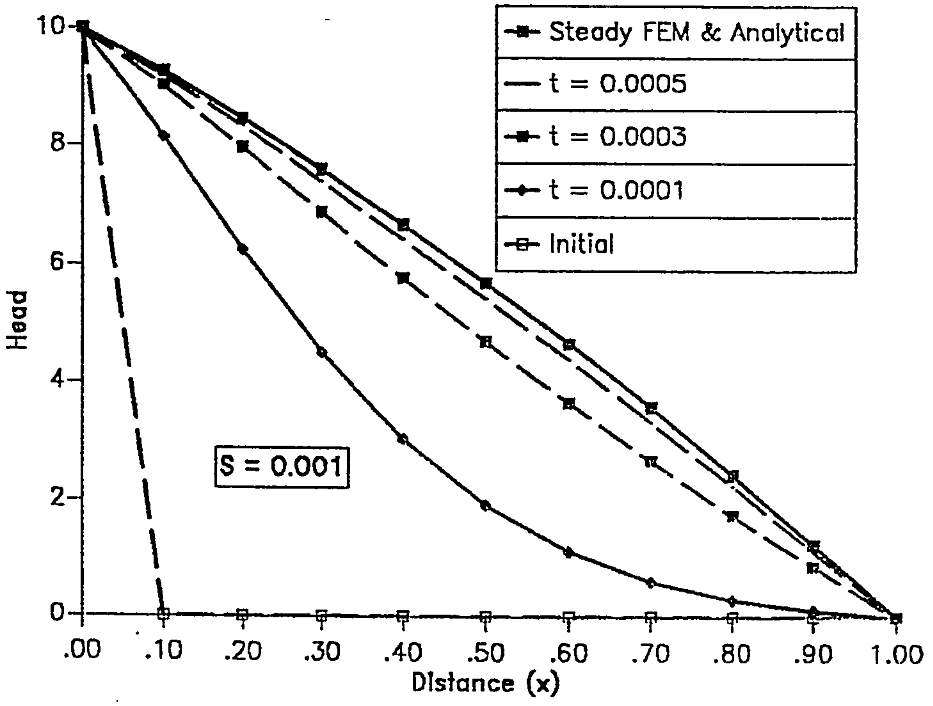


Figure-5.5c: Comparison of numerical and analytical solutions for transient groundwater flow equation for heterogeneous medium ($K = f = \frac{1}{1+x}$).

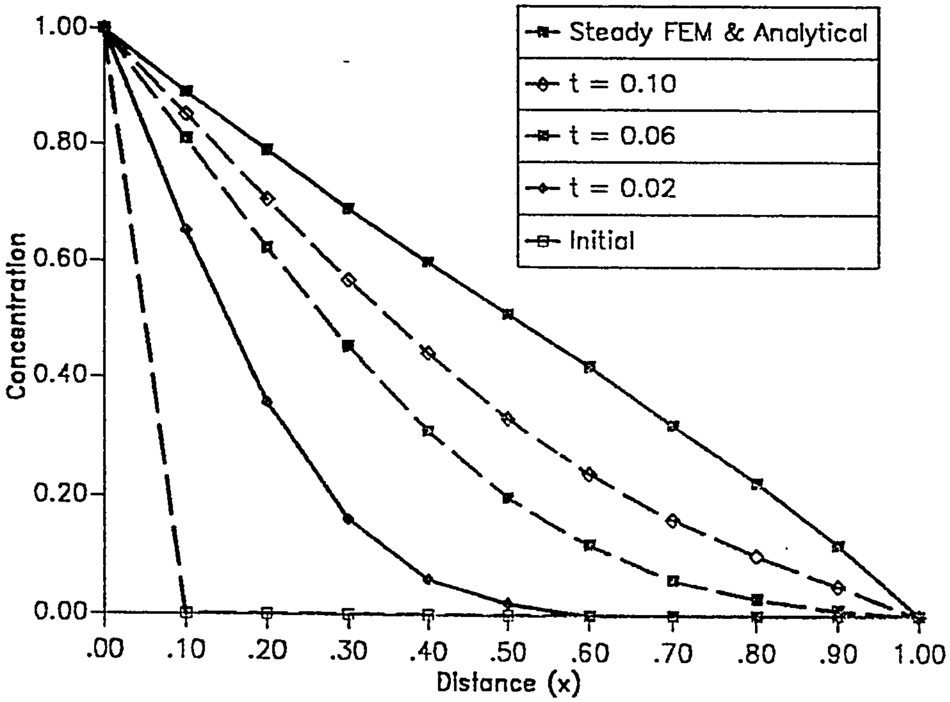


Figure-5.5d: Comparison of numerical and analytical solutions for transient solute transport equation for heterogeneous medium ($D = V = \frac{1}{1+x}$ and $f = \frac{4+2x}{(1+x)^2}$)

5.3 NUMERICAL STUDY OF SOLUTE AGGRESSIVENESS PHENOMENA

The developed model is applied to general cases illustrated in figure-5.1 and figure-5.12a for one and two-dimensional studies. Different situations are considered which will be described in the following sections.

5.3.1 One-dimensional Study

The two equations are coupled and solved simultaneously for concentration-dependent model parameters (figure-5.6 and figure-5.8). Figure-5.7 shows the propagation pattern of induced heterogeneity in the medium for an arbitrary linear relationship between hydraulic conductivity and solute concentration ($K = K_0 + mC$). The coupled system is then solved for aggressive and non-aggressive case and the predicted values of the dependent variables and the model parameters are compared (figures-5.9). The numerical study showed significant changes in the head distribution pattern where the solute is aggressive (figure-5.9, figure-5.10 and figure-5.11).

The effect of solute aggressiveness on one-dimensional concentration profile is found to be dependent on the magnitude of diffusion coefficient at the steady state. This is because the ratio $\frac{VL}{D}$, known as Peclet Number, remains unchanged at the steady state condition for one-dimensional problems when the diffusion coefficient is smaller compared to mechanical dispersion (figure-5.9c). Comparison of head distribution patterns for concentration dependent parameters and the constant parameter models clearly illustrated the existence of incompressible unsteady flow in porous media when the solute is aggressive (figure-5.6d and figure-5.8d).

The effect of tortuosity function is illustrated in figure-5.11j and figure-5.11k for different values of the exponent 'r' in equation (19).

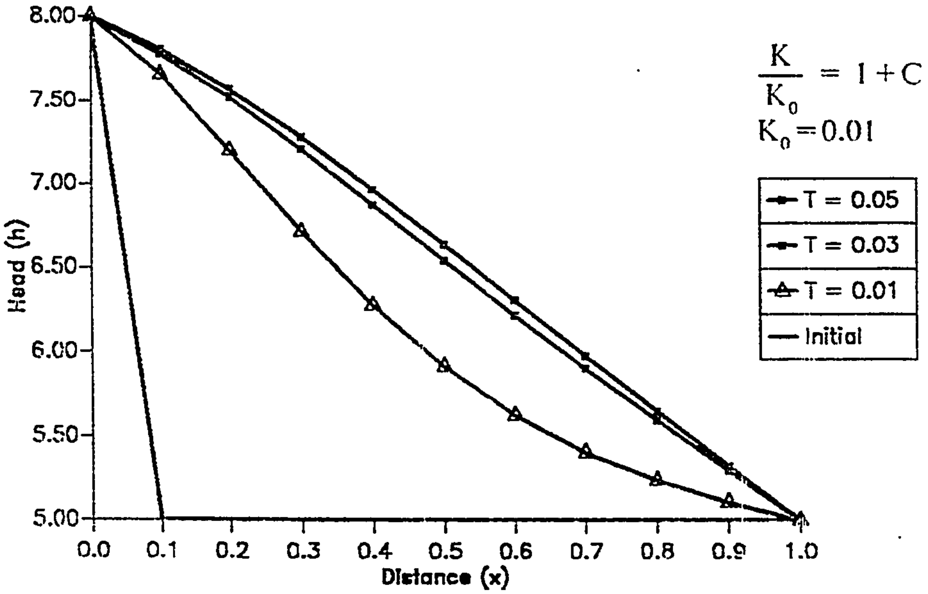


Figure-5.6a: Head distribution obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

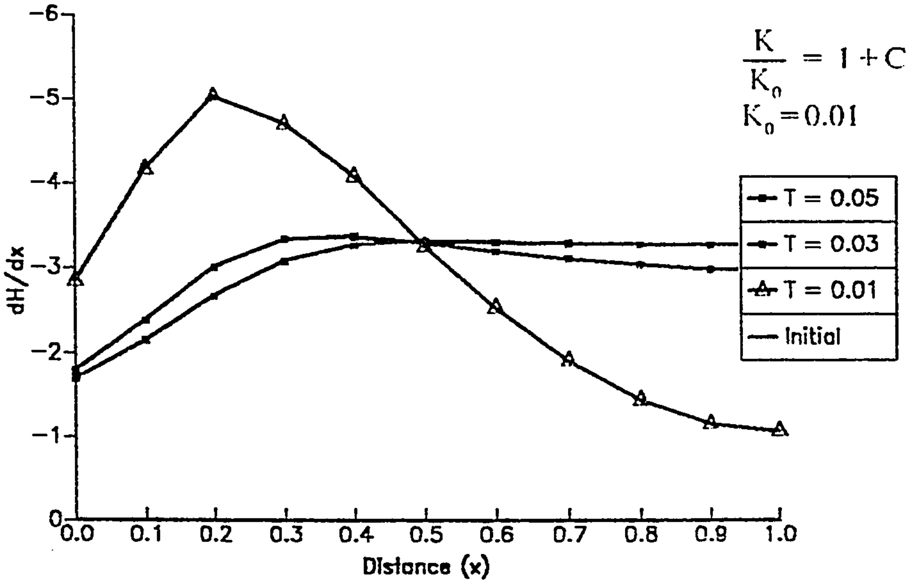


Figure-5.6b: Head gradient distribution obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

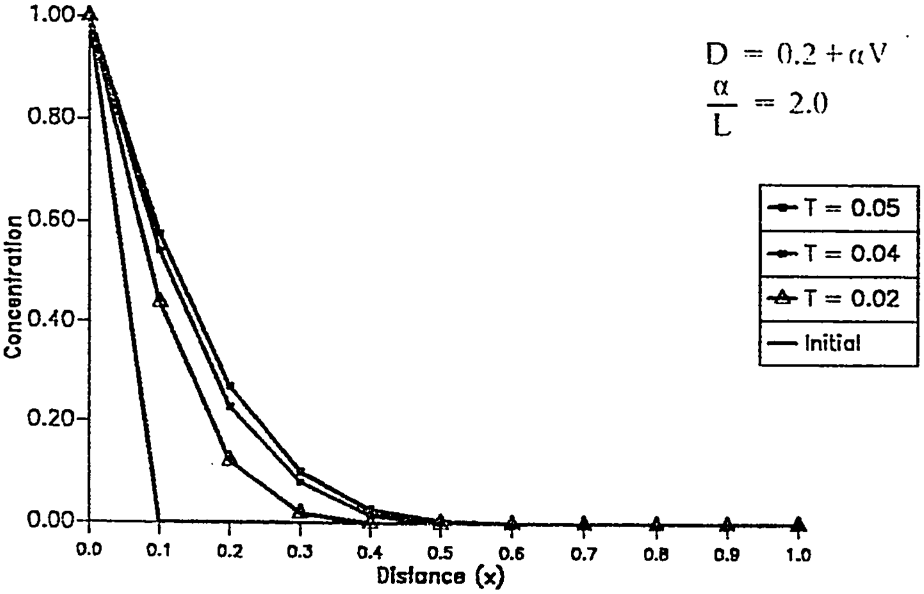


Figure-5.6c: Concentration distribution obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial\eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

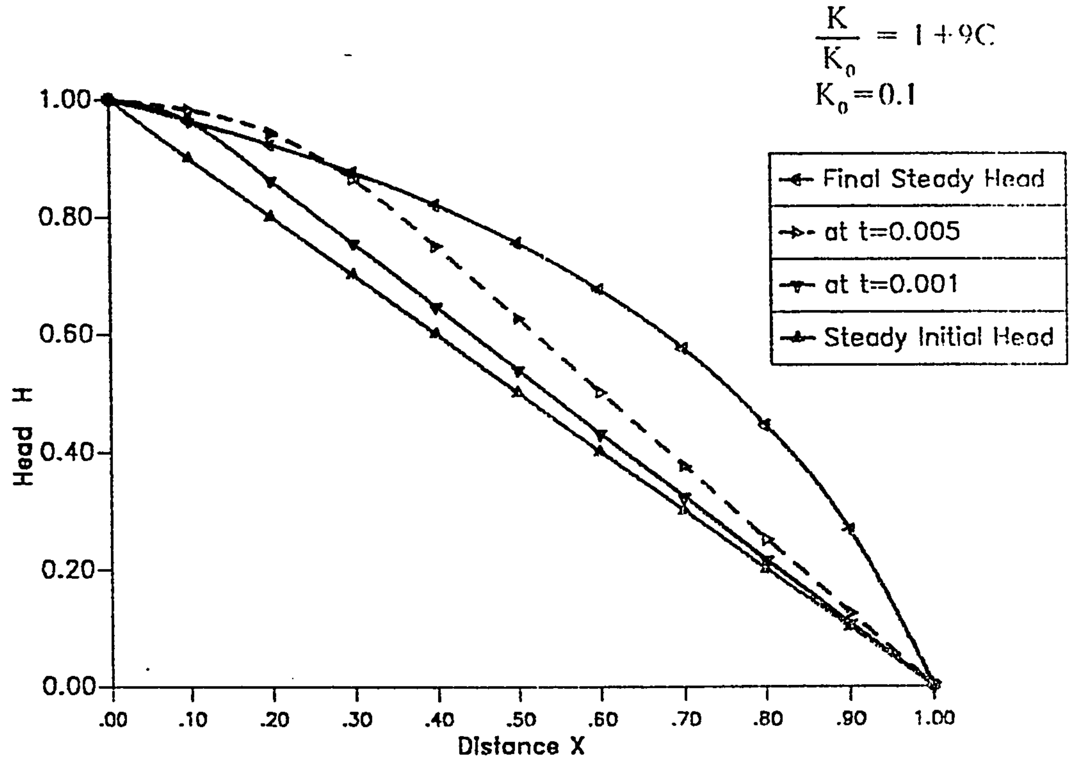


Figure-5.6d: Existence of incompressible unsteady flow . obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial\eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

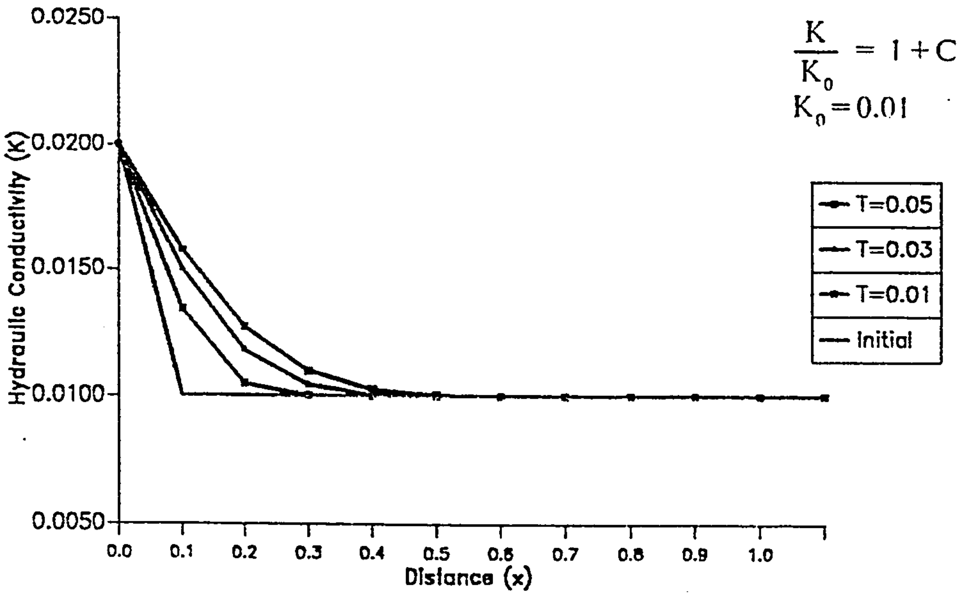


Figure-5.7a: Propagation of medium heterogeneity in terms of hydraulic conductivity obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

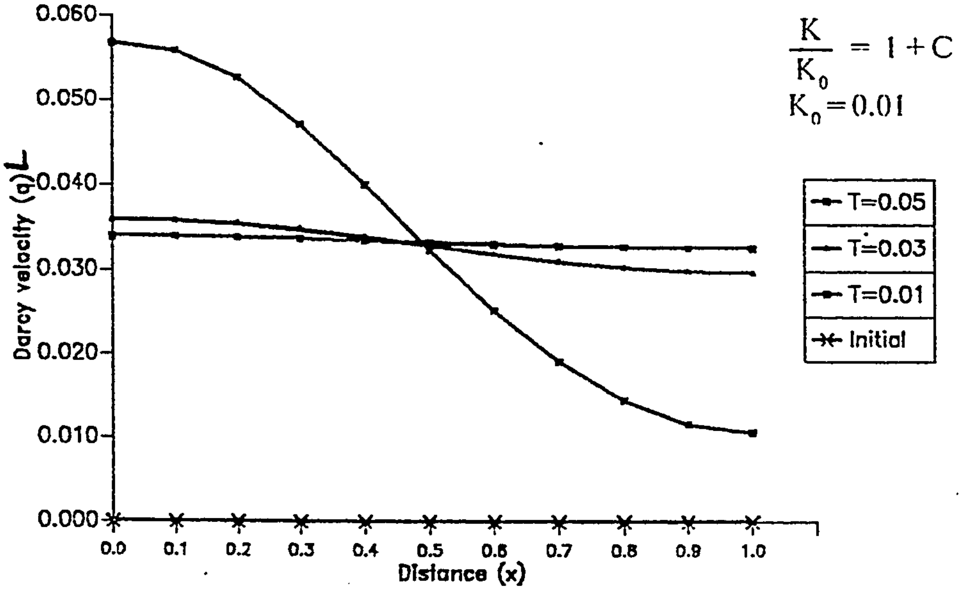


Figure-5.7b: Propagation of medium heterogeneity in terms of Darcy velocity obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial\eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

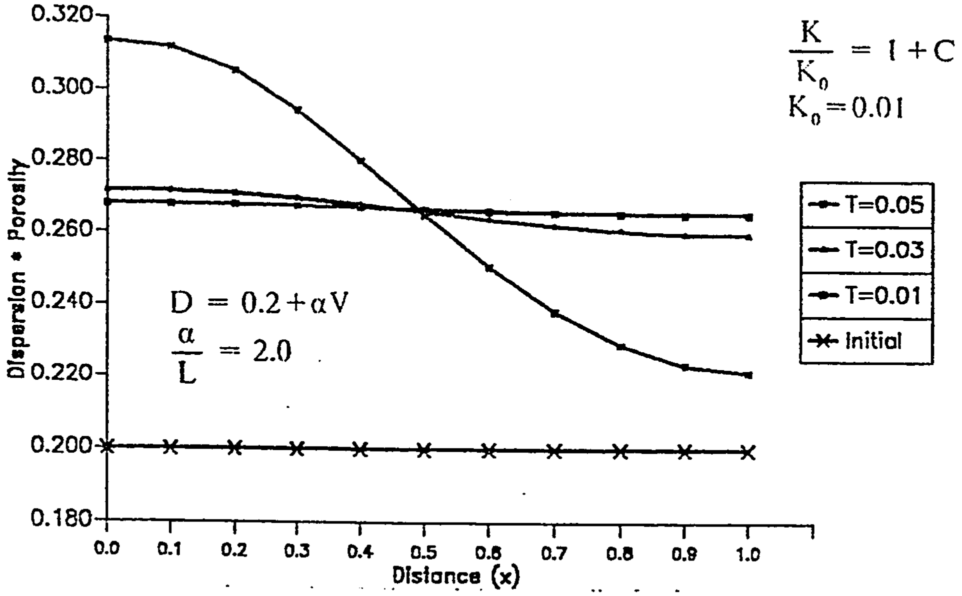


Figure-5.7c: Propagation of medium heterogeneity in terms of Dispersion coefficient obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

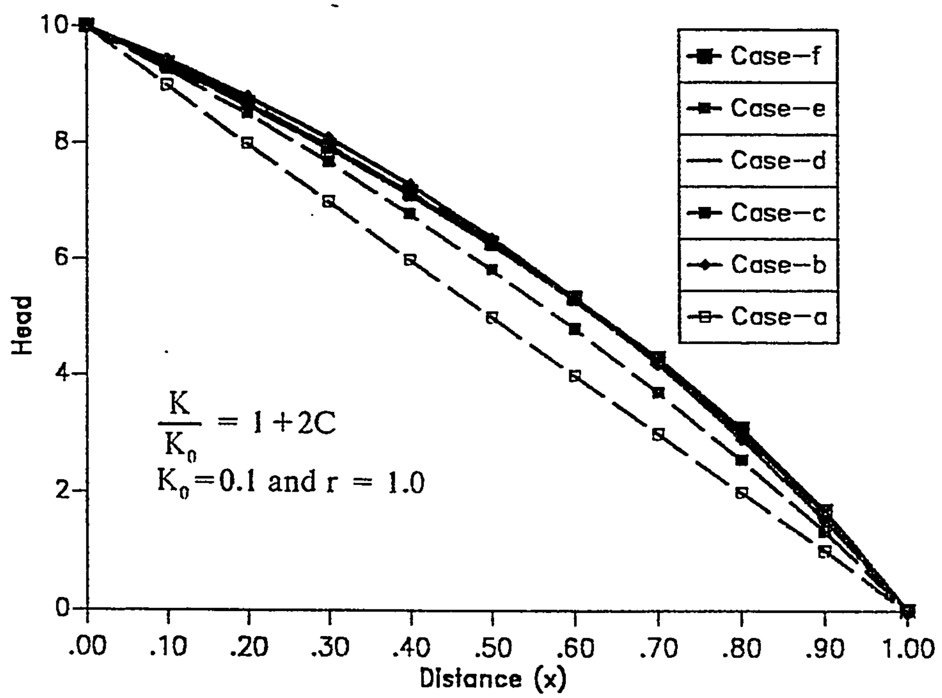


Figure-5.8a: Head distributions obtained from coupled solution for constant and concentration-dependent hydraulic conductivity for Fresh Aquifer:

a) Constant parameters at t = 0.01, 0.02 and steady

b) concentration-dependent with constant porosity at t = 0.01

c) concentration-dependent with variable porosity at t = 0.01

d) concentration-dependent with constant porosity at t = 0.02

e) concentration-dependent with variable porosity at t = 0.02

f) concentration-dependent at steady state

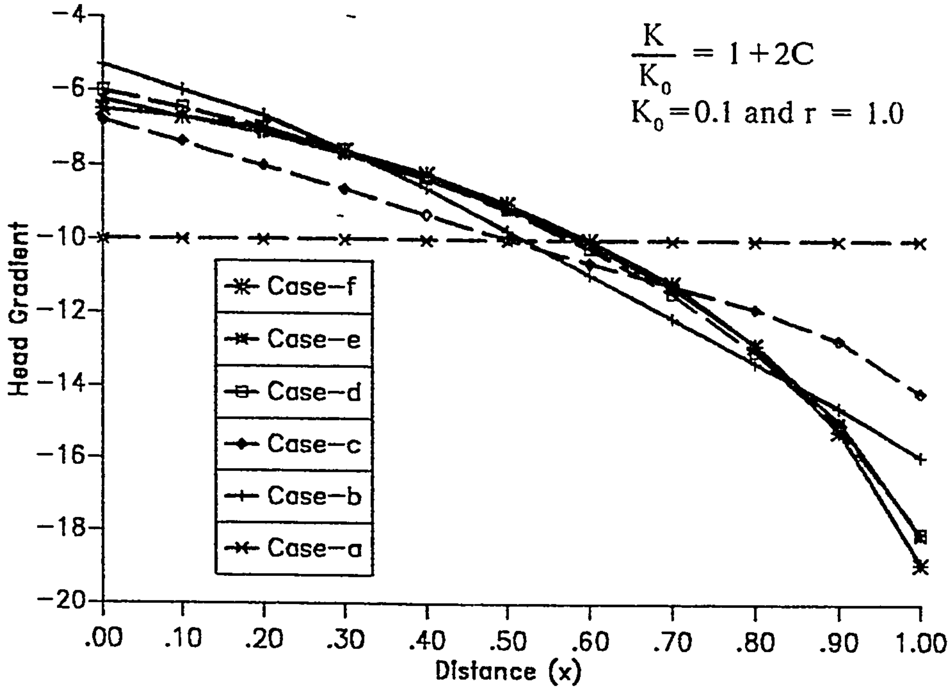


Figure-5.8b: Head gradient distributions obtained from coupled solution for constant and concentration-dependent hydraulic conductivity for Fresh Aquifer : a) Constant parameters at t = 0.01, 0.02 and steady b) concentration-dependent with constant porosity at t = 0.01 c) concentration-dependent with variable porosity at t = 0.01 d) concentration-dependent with constant porosity at t = 0.02 e) concentration-dependent with variable porosity at t = 0.02 f) concentration-dependent at steady state

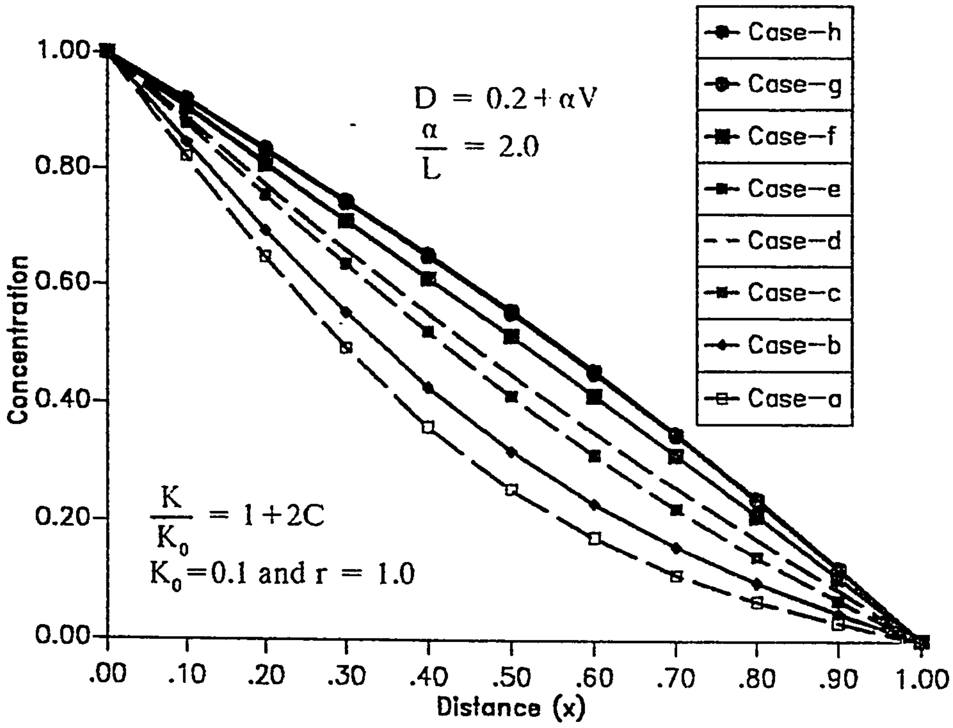


Figure-5.8c: Concentration distributions obtained from coupled solution for constant and concentration-dependent hydraulic conductivity for Fresh Aquifer: a) Constant parameters at t = 0.01

b) concentration-dependent with constant porosity at t = 0.01

c) concentration-dependent with variable porosity at t = 0.01

d) Constant parameters at t = 0.02

e) concentration-dependent with constant porosity at t = 0.02

f) concentration-dependent with variable porosity at t = 0.02

g) Constant parameters at steady state

h) concentration-dependent at steady state

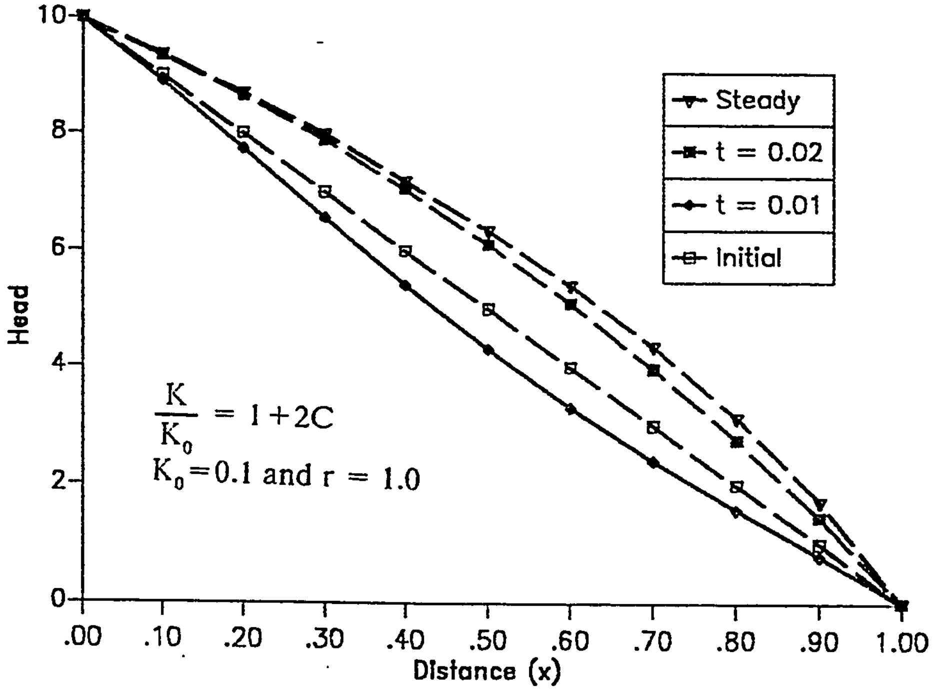


Figure-5.8d: Existence of incompressible unsteady flow , obtained from coupled solution for concentration-dependent hydraulic conductivity considering $(\frac{\partial\eta}{\partial t})_{s.a.}$ (Fresh Aquifer)

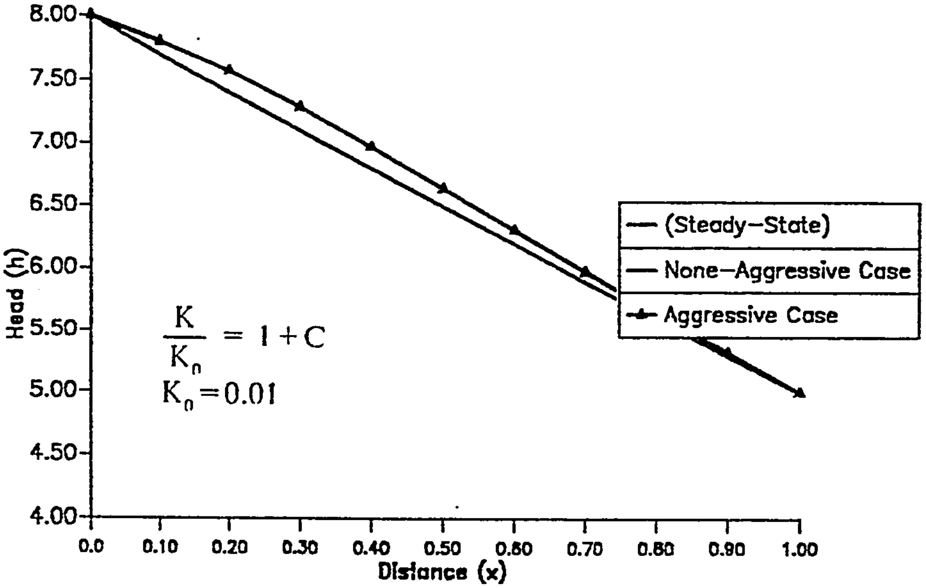


Figure-5.9a: Comparison of Steady head distribution for aggressive and non-aggressive cases (fresh aquifer)

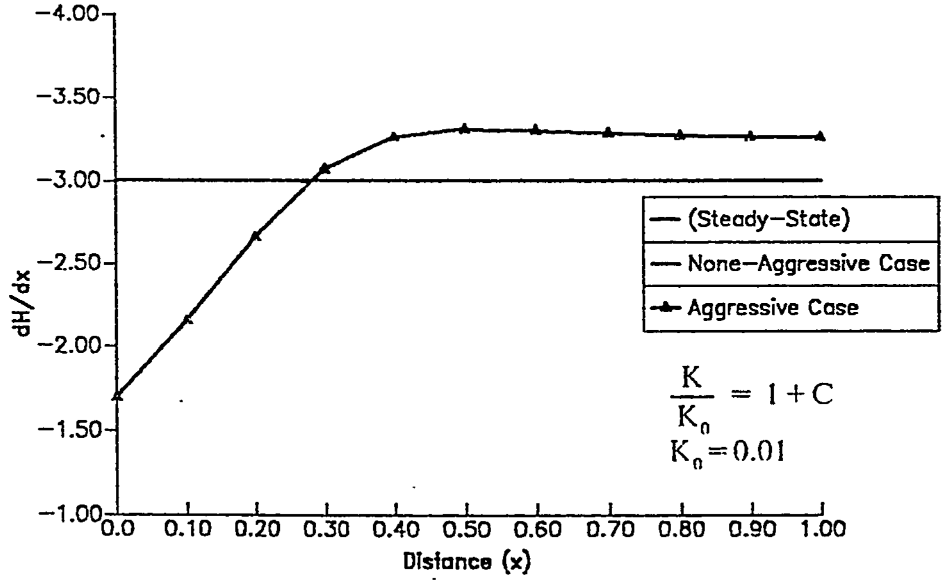


Figure-5.9b: Comparison of Steady head gradient distribution for aggressive and non-aggressive cases (fresh aquifer)

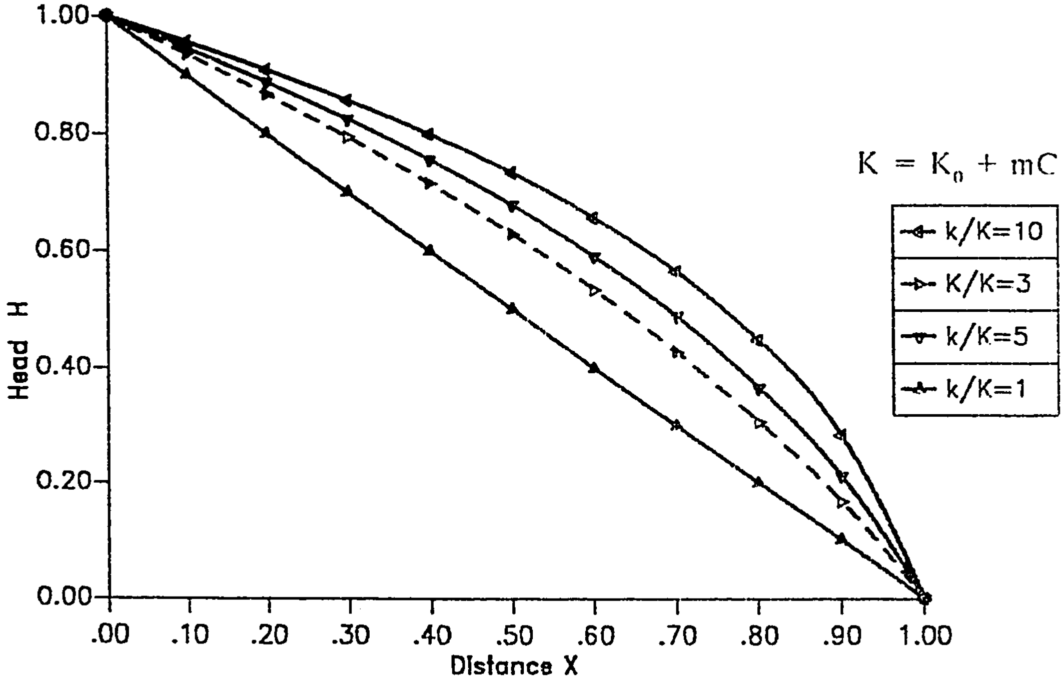


Figure-5.9c: Study of the effects of solute aggressiveness on steady head distribution at different aggressiveness levels (fresh aquifer)

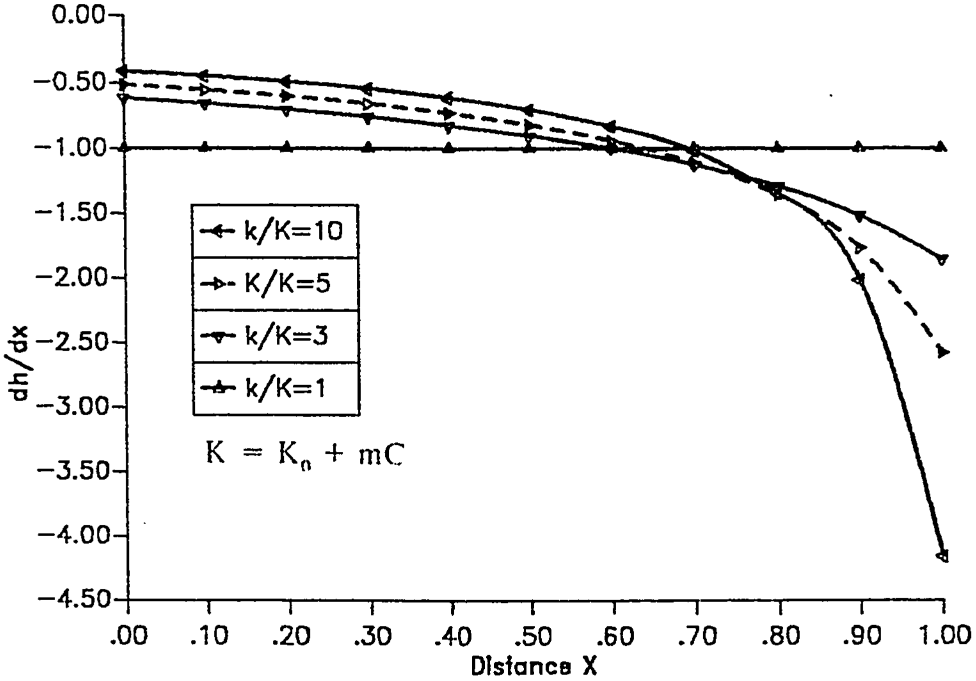


Figure-5.9d: Study of the effects of solute aggressiveness on steady head gradient distribution at different aggressiveness levels (fresh aquifer)

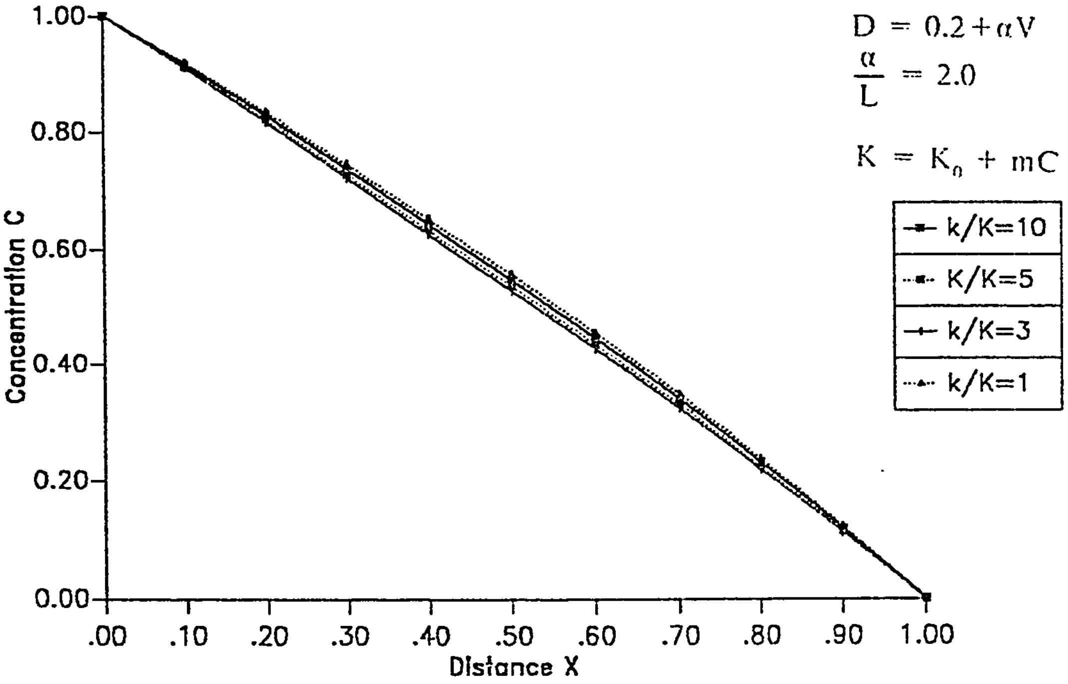


Figure-5.9c: Study of the effects of solute aggressiveness on steady concentration distribution at different aggressiveness levels (fresh aquifer)

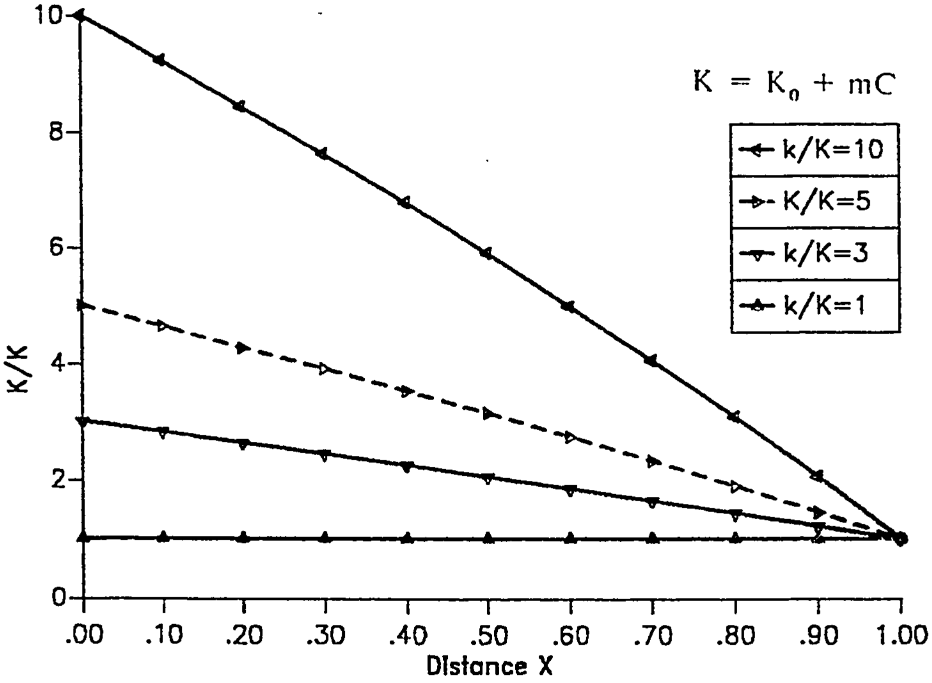


Figure-5.9f: Study of the effects of solute aggressiveness on model parameters at different aggressiveness levels (fresh aquifer)

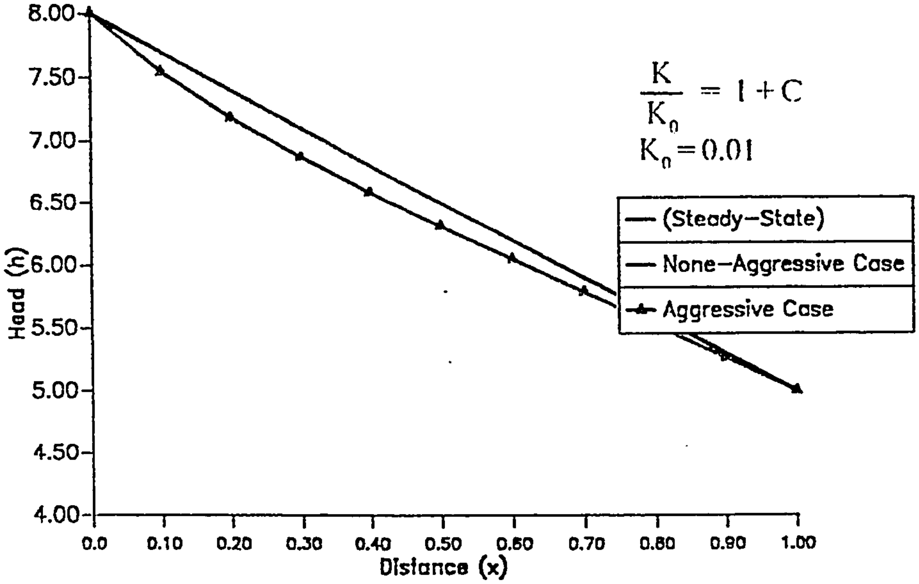


Figure-5.10a: Comparison of Steady head distribution for aggressive and non-aggressive cases (contaminated aquifer)

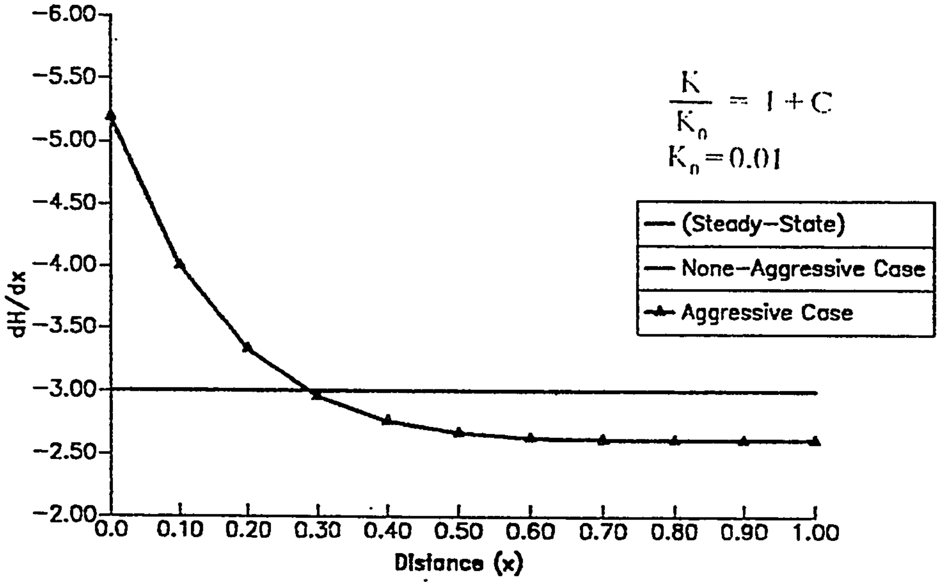


Figure-5.10b: Comparison of Steady head gradient distribution for aggressive and non-aggressive cases (contaminated aquifer)

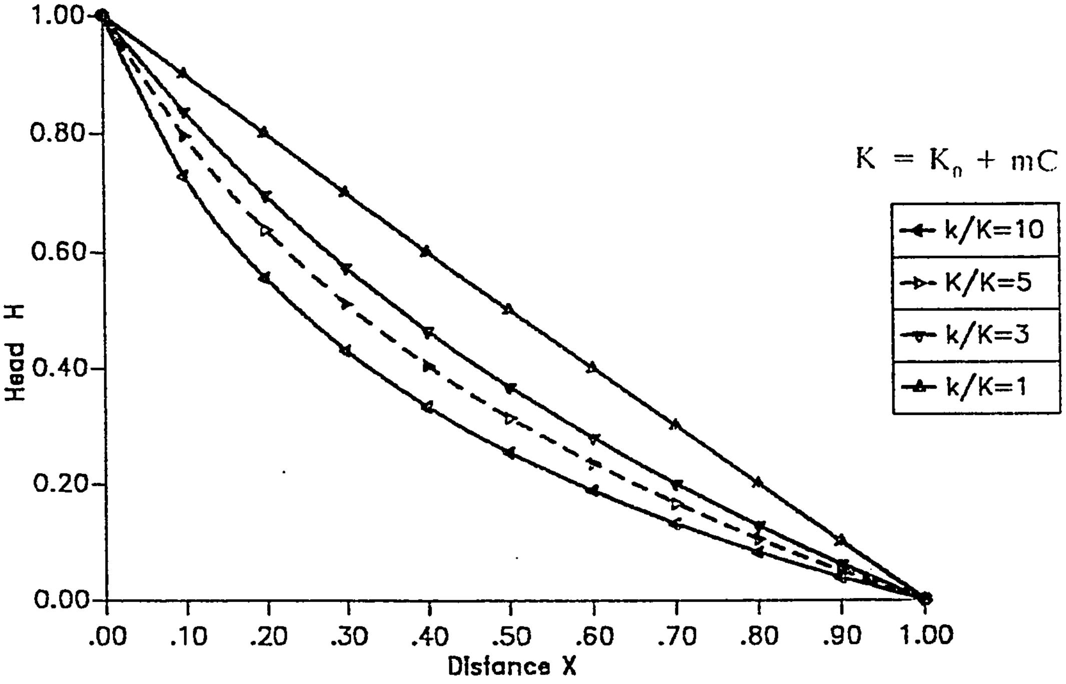


Figure-5.11a: Study of the effects of solute aggressiveness on steady head distribution at different aggressiveness levels (contaminated aquifer)

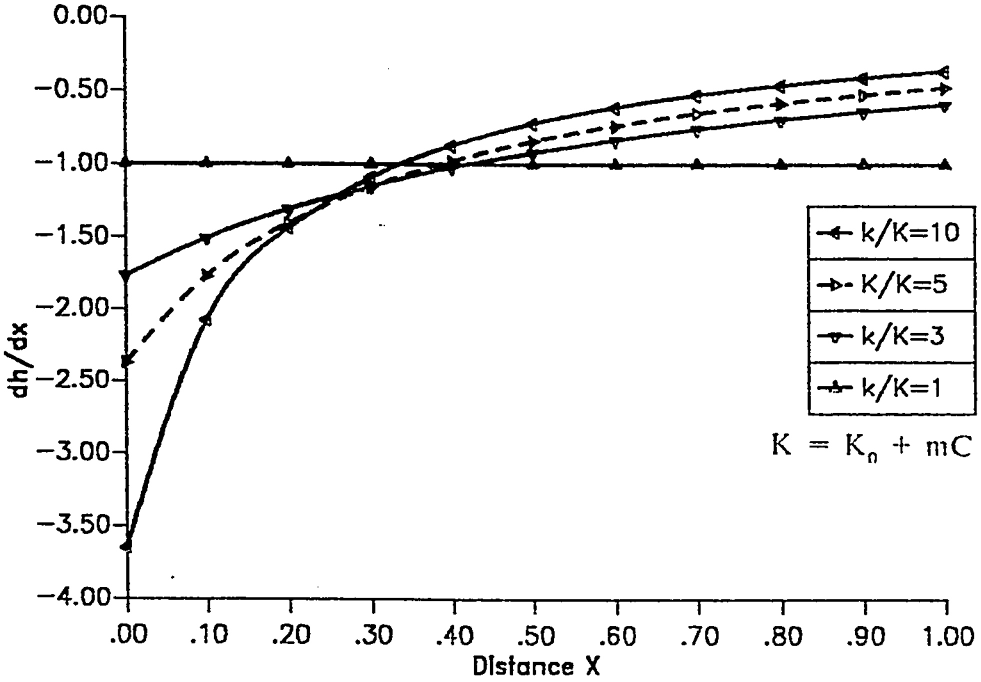


Figure-5.11b: Study of the effects of solute aggressiveness on steady head gradient distribution at different aggressiveness levels (contaminated aquifer)

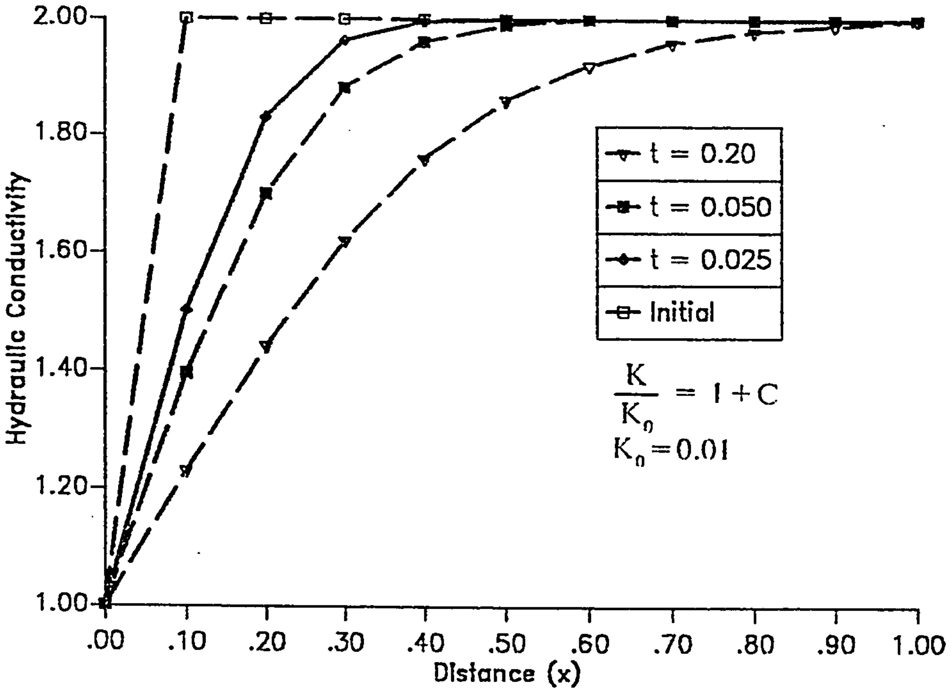


Figure-5.11c: Propagation of medium heterogeneity in terms of hydraulic conductivity obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Contaminated Aquifer)

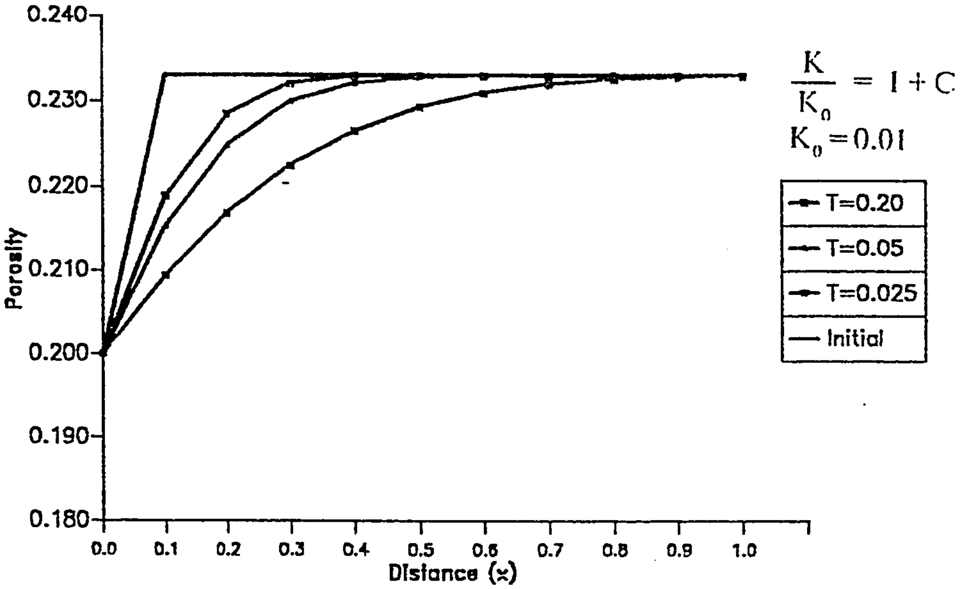


Figure-5.11d: Propagation of medium heterogeneity in terms of porosity obtained from coupled solution for concentration-dependent hydraulic conductivity without considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ (Contaminated Aquifer)

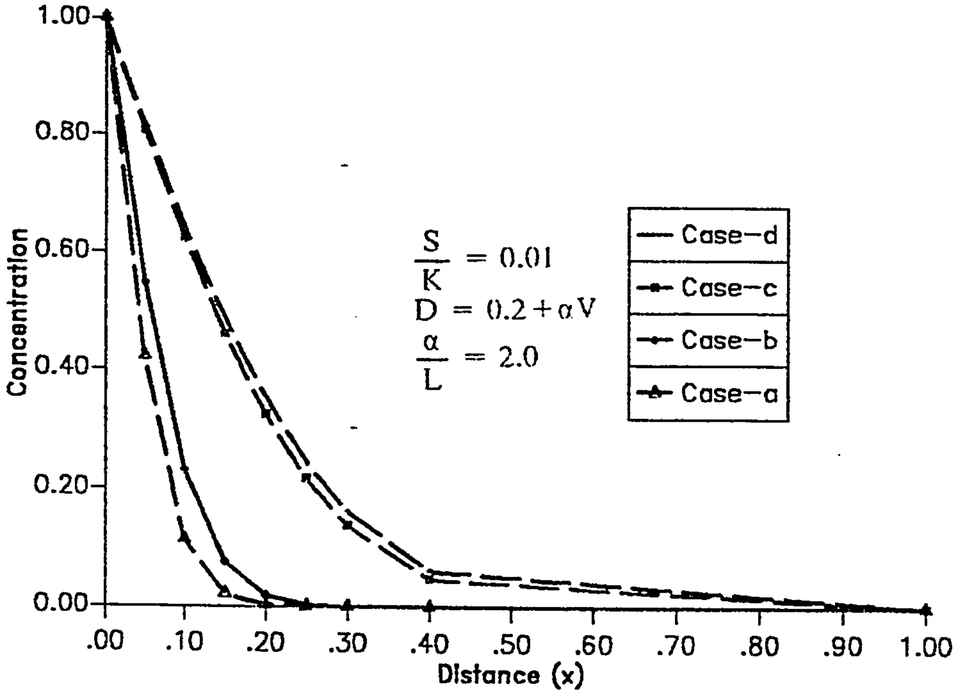


Figure-5.11c: Comparison of transient concentration distribution for uniform groundwater flow (conventional) and transient groundwater flow (coupled, non-aggressive) : a) uniform velocity at t =0.001 b) transient flow at t = 0.001 c) uniform velocity at t =0.01 d) transient flow at t = 0.01

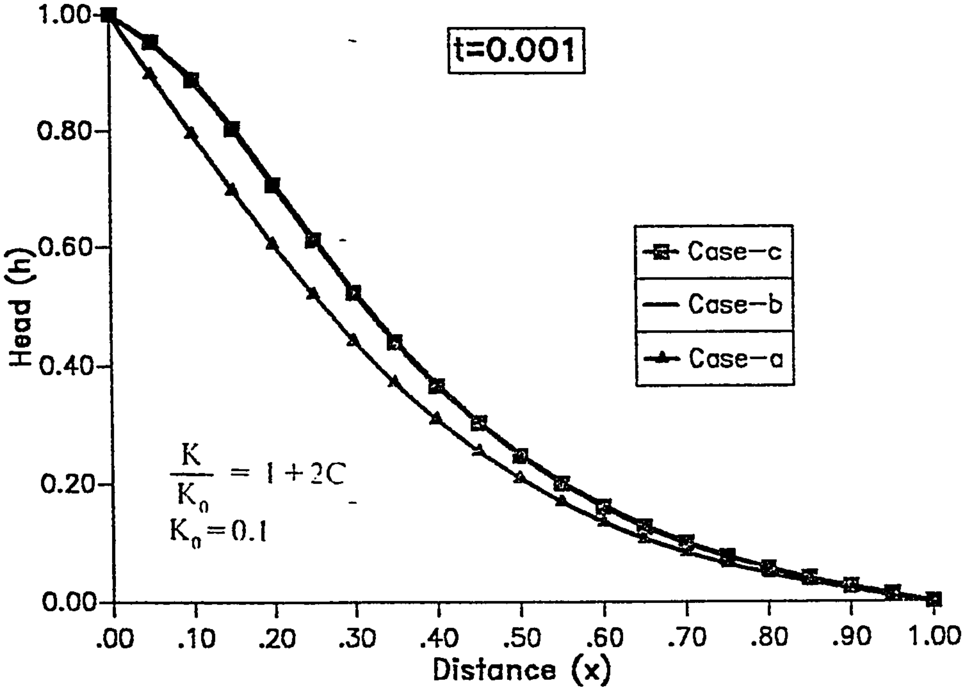


Figure-5.11f: Comparison of transient head distribution for constant and concentration-dependent parameters at $t=0.001$: a) constant parameters b) concentration-dependent with constant porosity c) concentration-dependent considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ with a factor less than unity

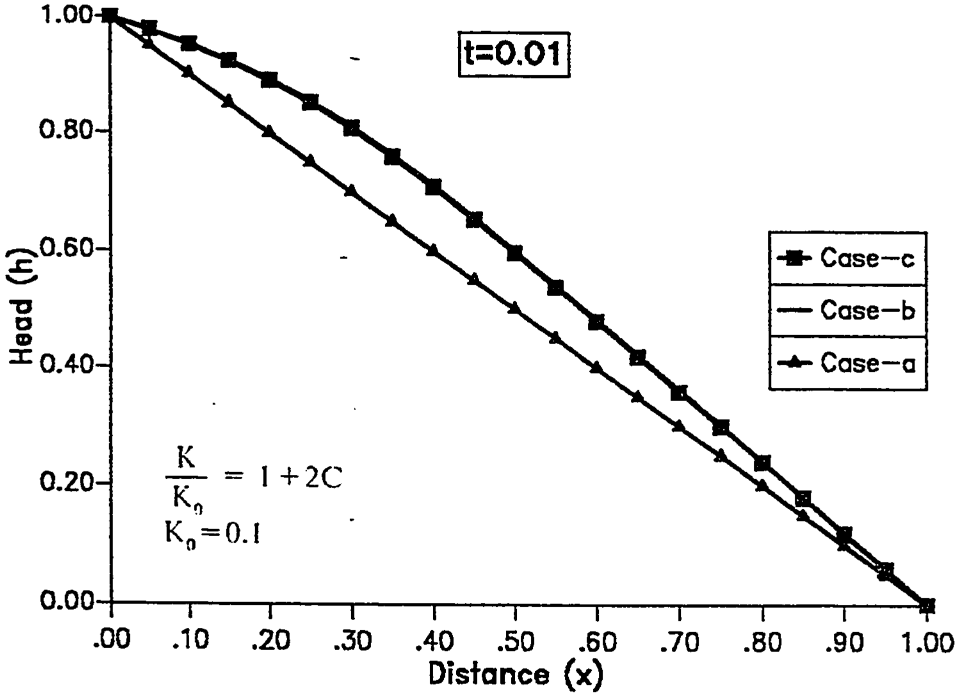


Figure-5.11g: Comparison of transient head distribution for constant and concentration-dependent parameters at $t=0.01$: a) constant parameters b) concentration-dependent with constant porosity c) concentration-dependent considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ with a factor less than unity

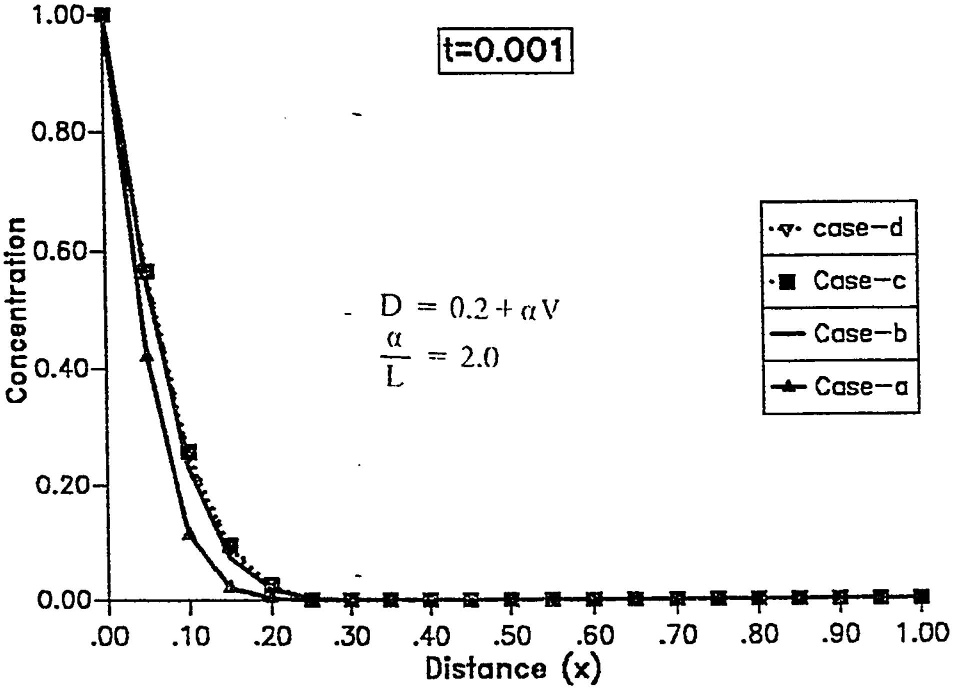


Figure-5.11h: Comparison of transient concentration distribution for constant and concentration-dependent parameters at t=0.001: a) constant parameters uniform velocity a) constant parameters transient velocity c) concentration-dependent with constant porosity d) concentration-dependent considering $(\frac{\partial\eta}{\partial t})_{s.a.}$ with a factor less than unity

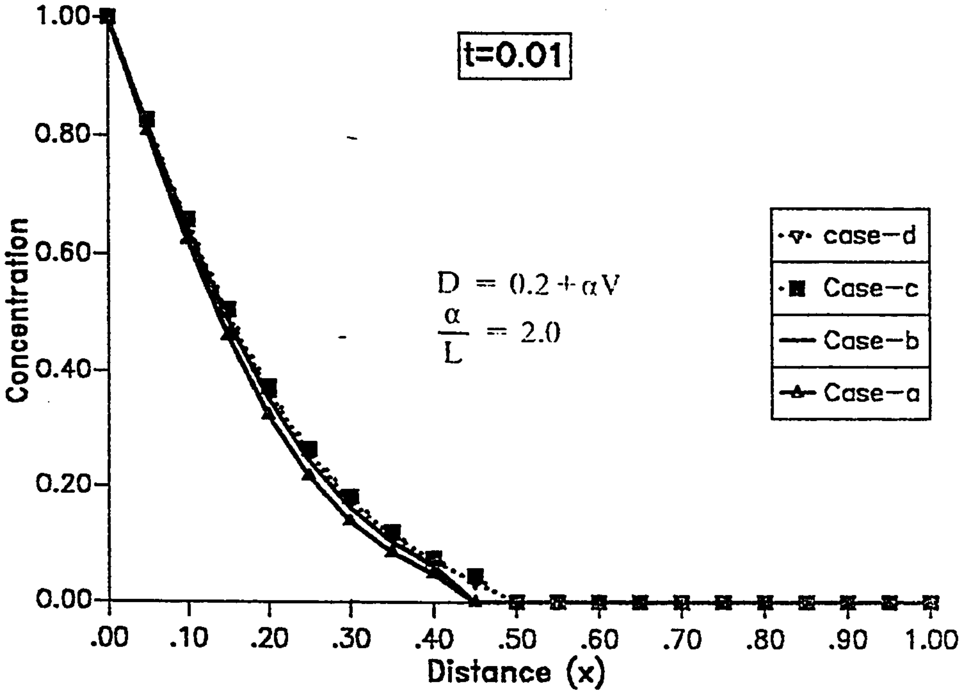


Figure-5.11i: Comparison of transient concentration distribution for constant and concentration-dependent parameters at t = 0.01: a) constant parameters uniform velocity a) constant parameters transient velocity c) concentration-dependent with constant porosity d) concentration-dependent considering $(\frac{\partial \eta}{\partial t})_{s.a.}$ with a factor less than unity

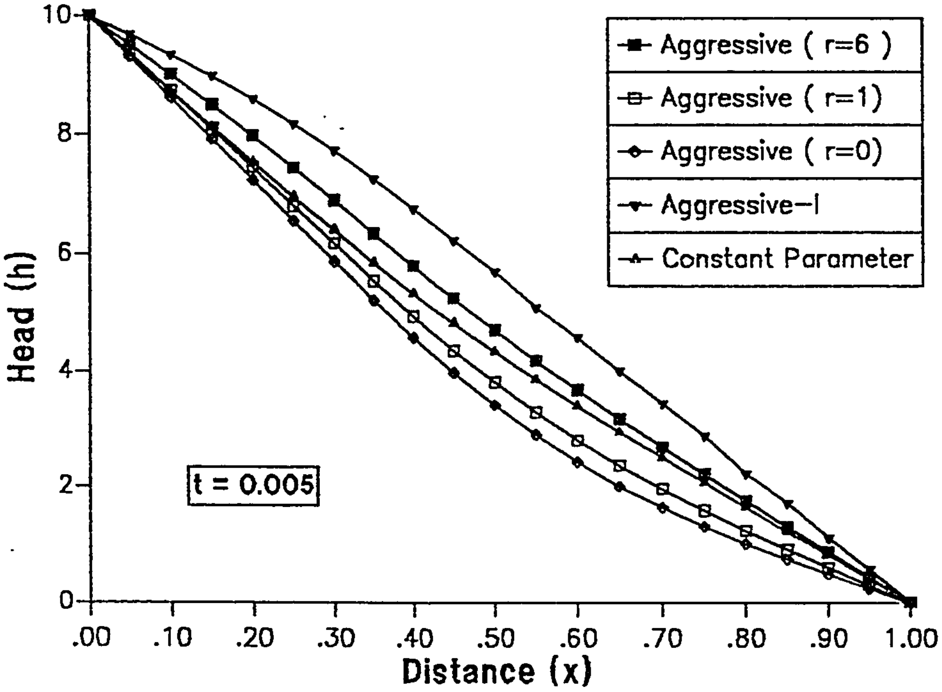


Figure-5.11j: Effect of r on transient Head distribution for concentration-dependent parameters

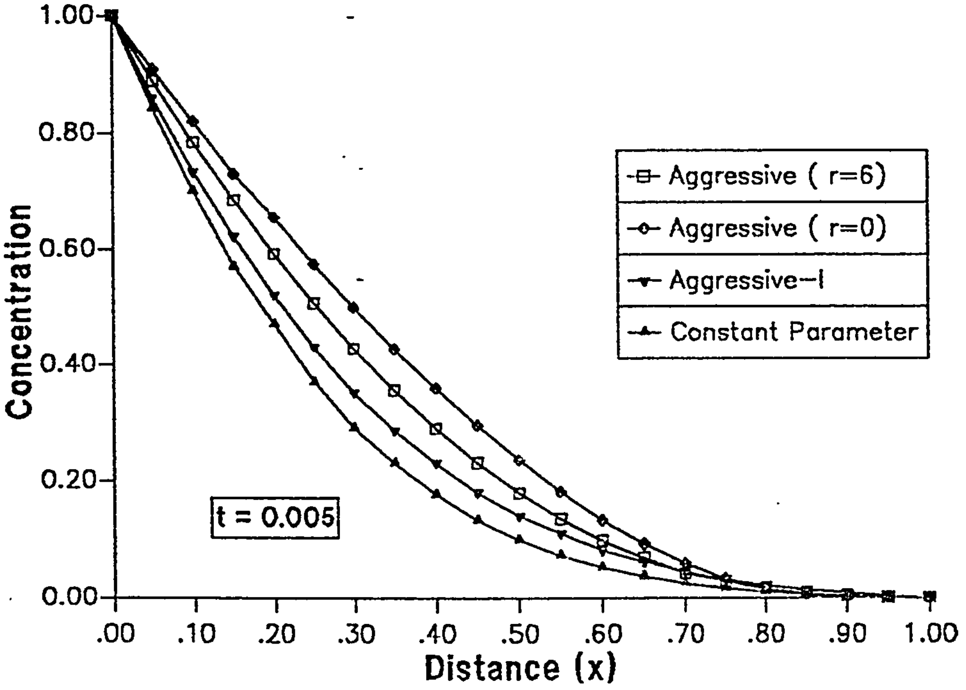


Figure-5.11k: Effect of r on transient concentration distribution for concentration-dependent parameters

5.3.2 Two-dimensional Study

The two dimensional test problems solved here are the same problems used by Mohsen (1987) and Bhuiyan et. al.(1990). They solved the problem for one-dimensional uniform velocity field only, thereby solving only the transport equation (figure-5.12a).

The numerical model predictions for coupled system is presented in figures-5.13, 5.14, 5.15 and 5.17. The simultaneous solution of the non-linear system showed significant variations in the head and the concentration distribution pattern (figures-5.18). The numerical study also showed the existence of incompressible unsteady groundwater flow for aggressive solutes (figure-5.19). The medium heterogeneity induced due to solute aggressiveness phenomena is shown in figures-5.16a, 5.16b, 5.19c and 5.19d. An abritrary linear relationship between hydraulic conductivity and the solute concentration was used in two-dimensional simulation also. Any type of hydraulic conductivity-concentration relationship can be used in the model by modifying the function subroutine only.

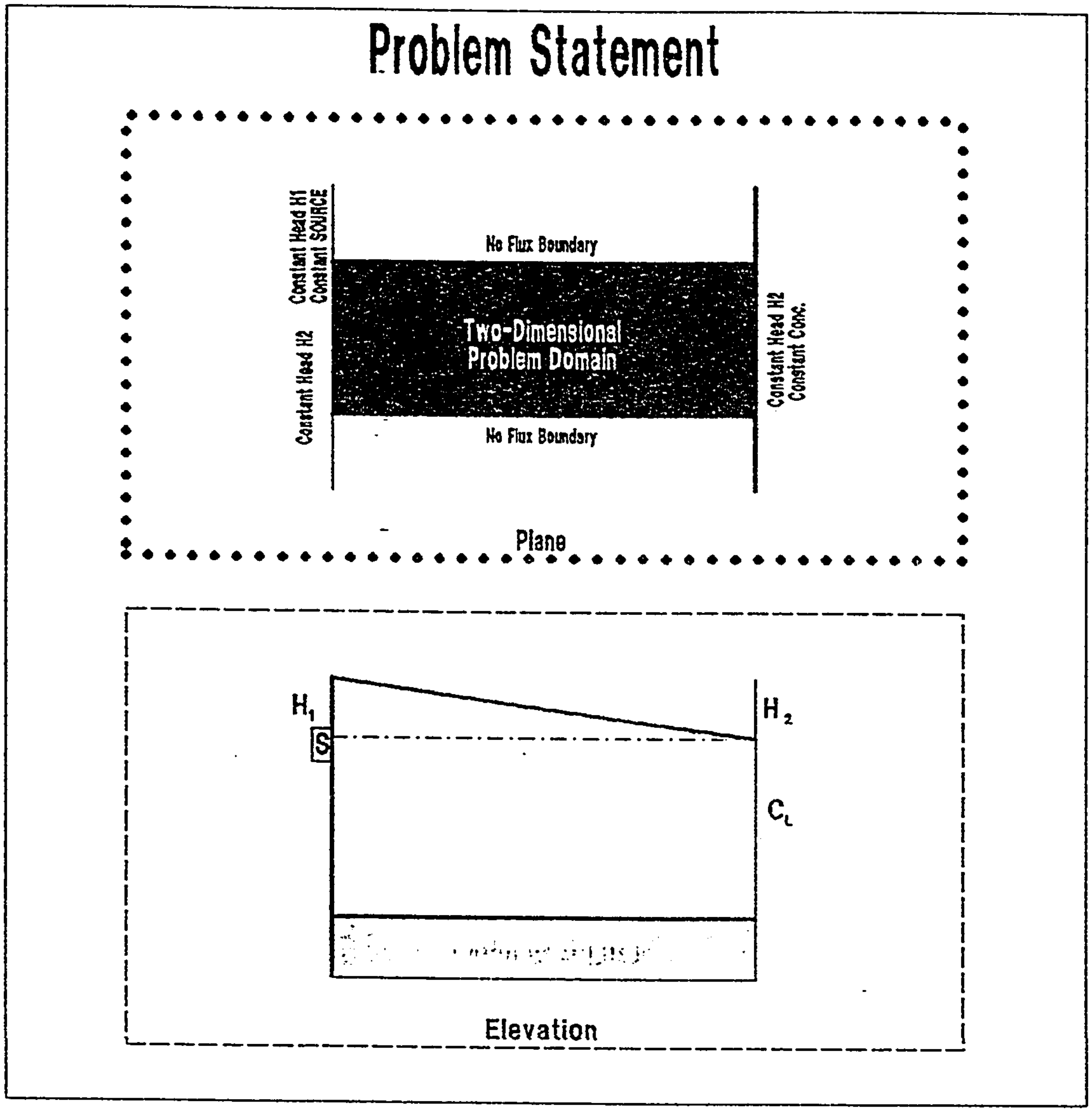


Figure-5.12a: Problem statement in Two-dimensional Analysis

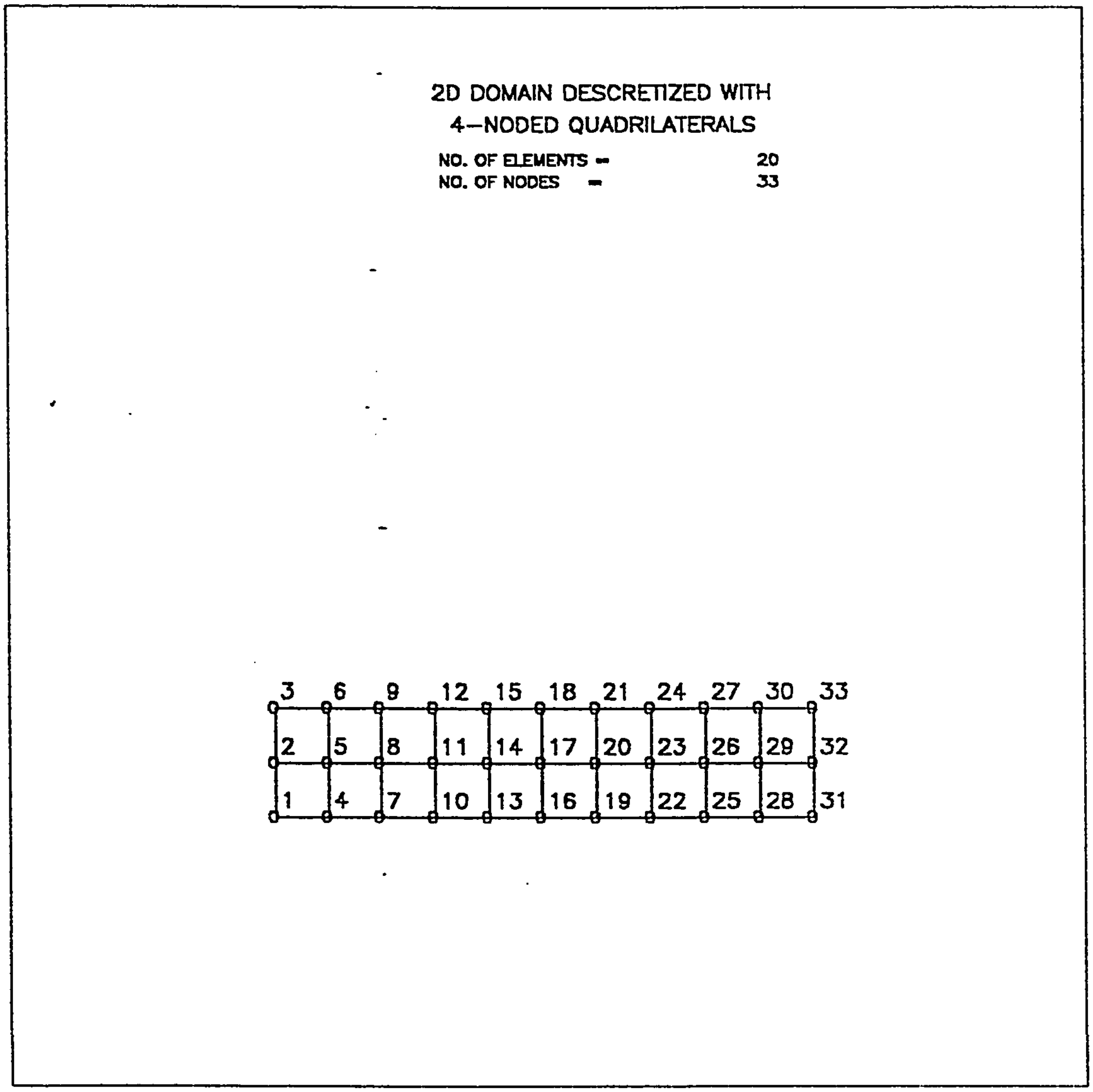


Figure-5.12b:Two-dimensional mesh for virtually one-dimensional Analysis

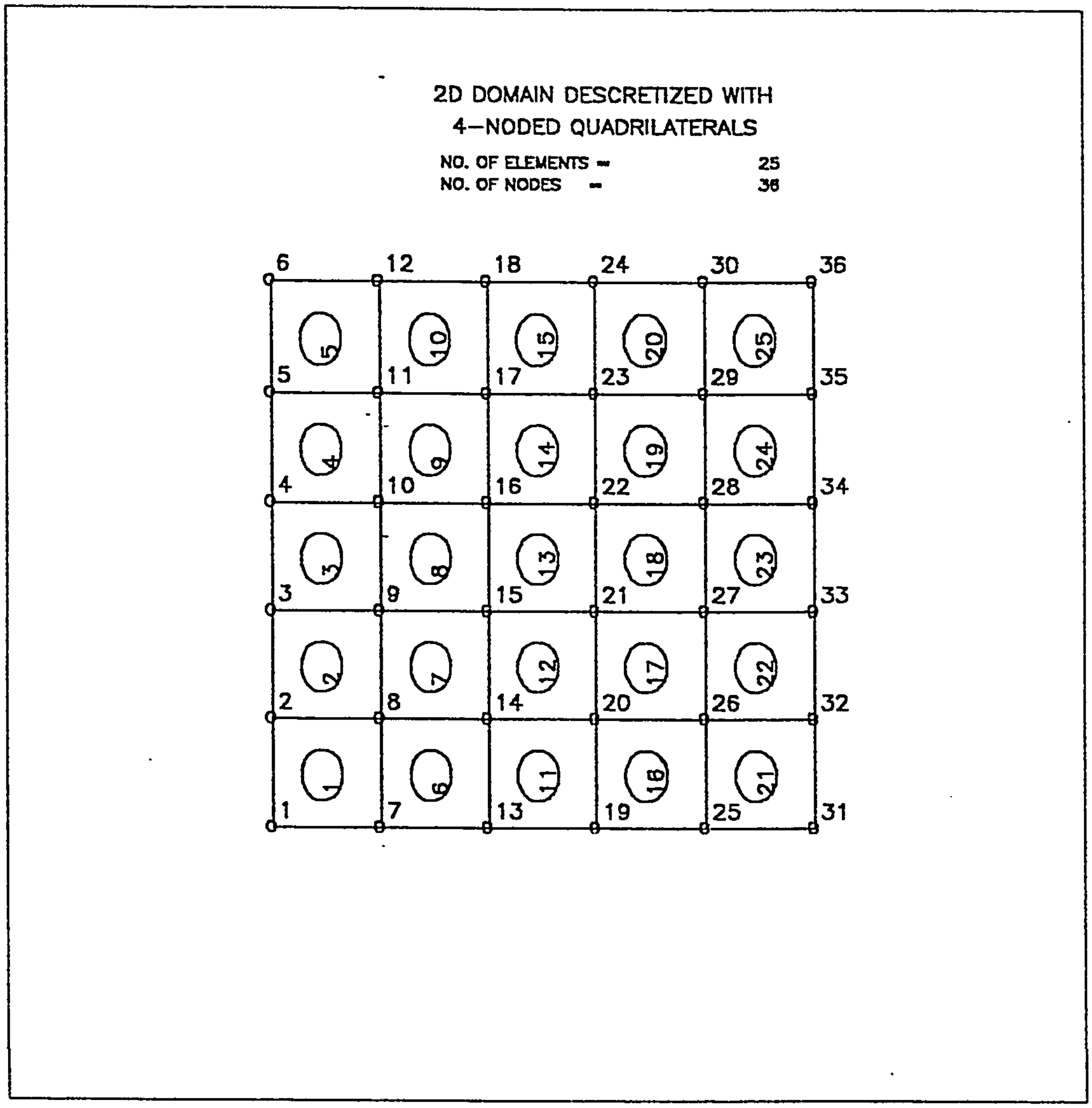


Figure-5.12c: Two-dimensional mesh for Two-dimensional Analysis

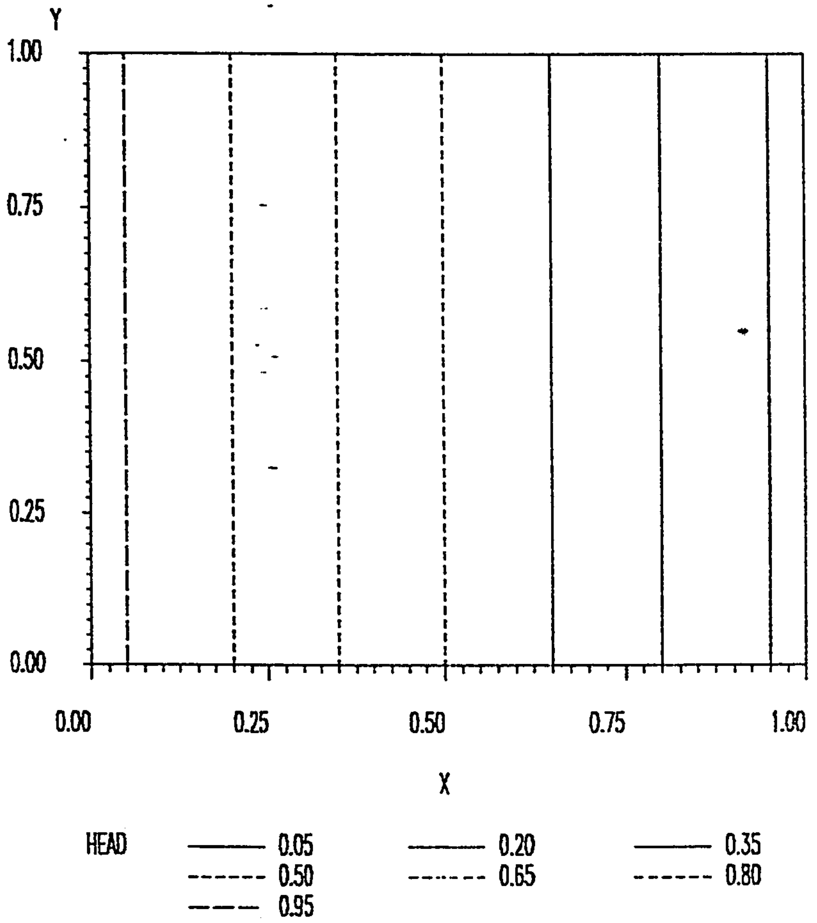


Figure-5.13a: Constant parameter Steady Two-dimensional Head distribution for virtually one-dimensional problem (Numerical results matching the analytical one)

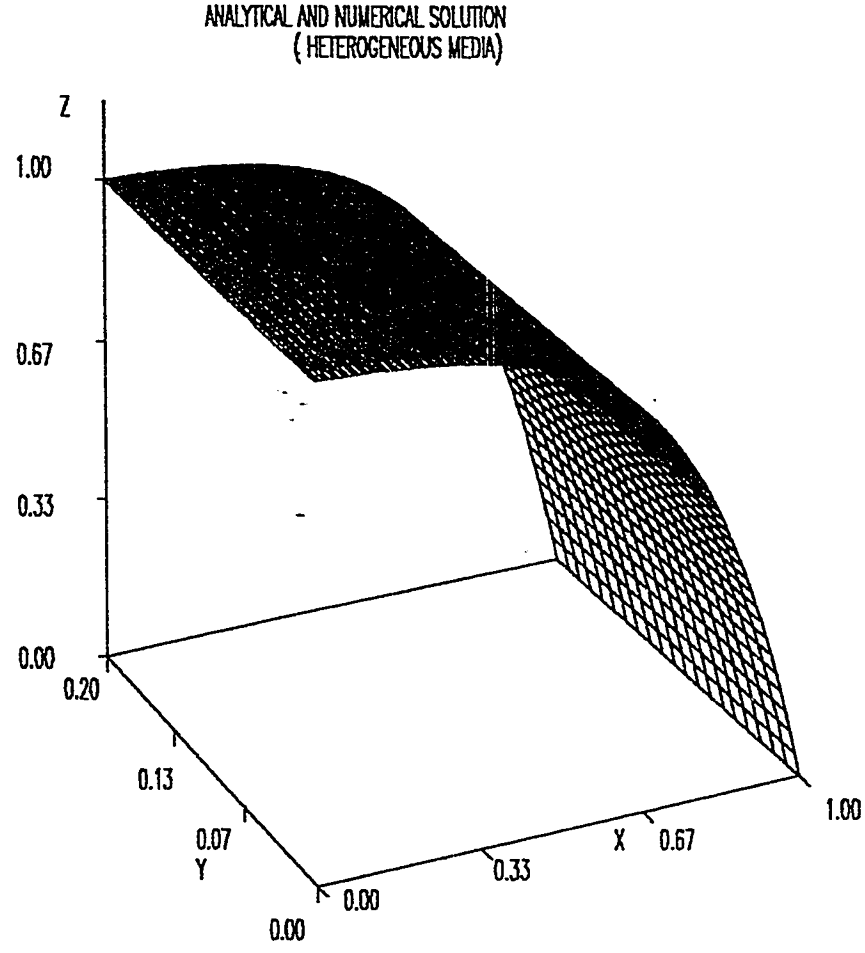


Figure-5.13b: Constant parameter steady concentration distribution in two-dimensional space for virtually one-dimensional problem (Numerical results matching the analytical one)

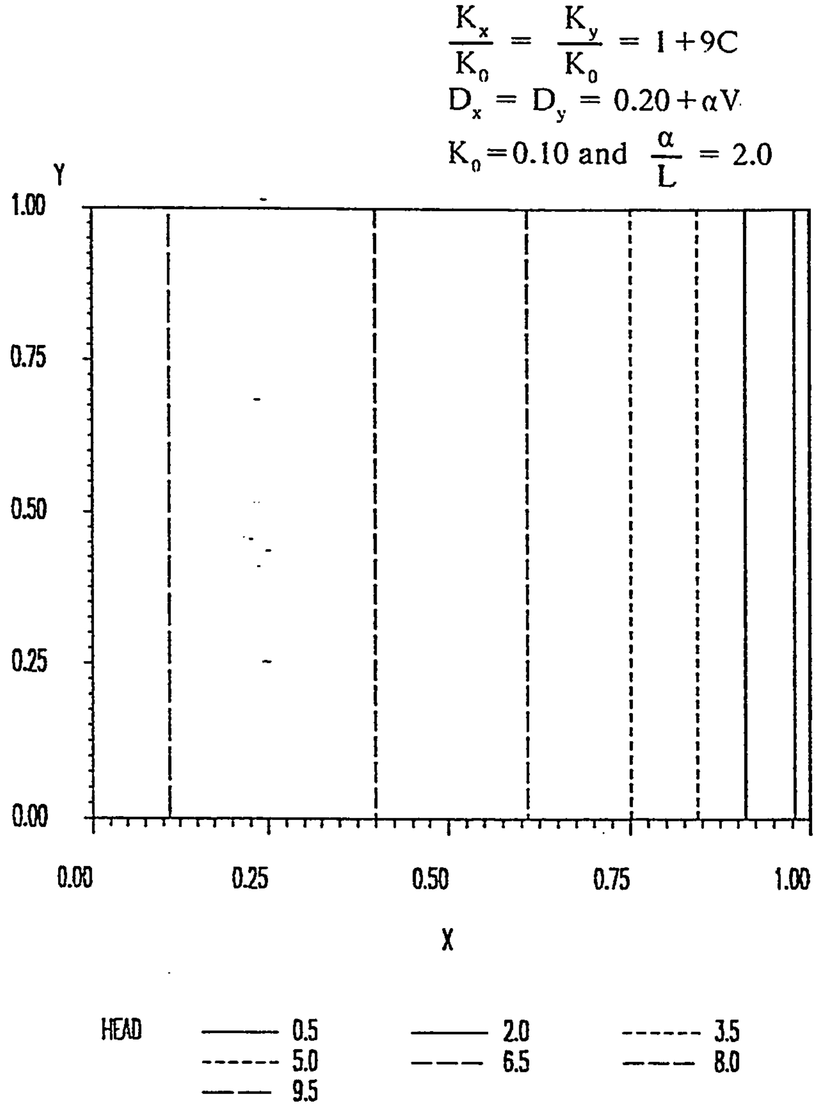


Figure-5.14a: Steady Two-dimensional Head distribution for virtually one-dimensional problem obtained from concentration-dependent parameters

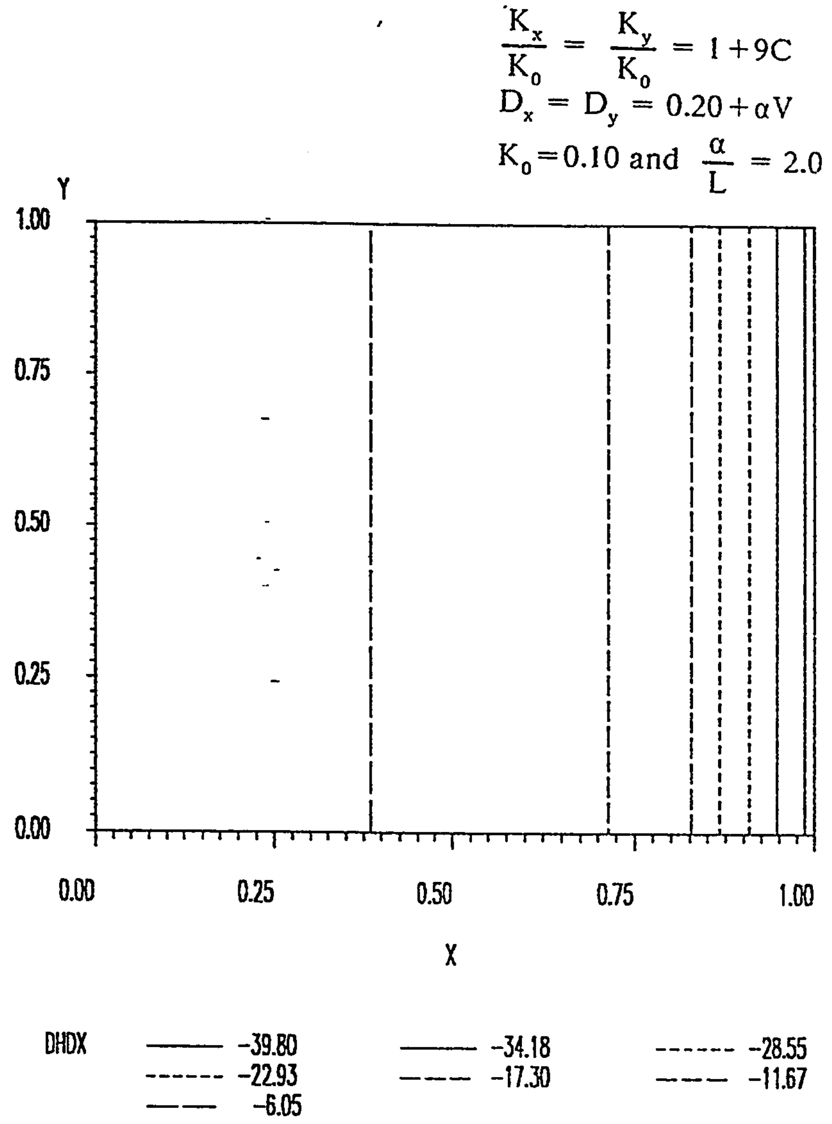


Figure-5.14b: Steady Head Gradient distribution in two-dimensional space for virtually one-dimensional problem obtained from concentration-dependent parameters

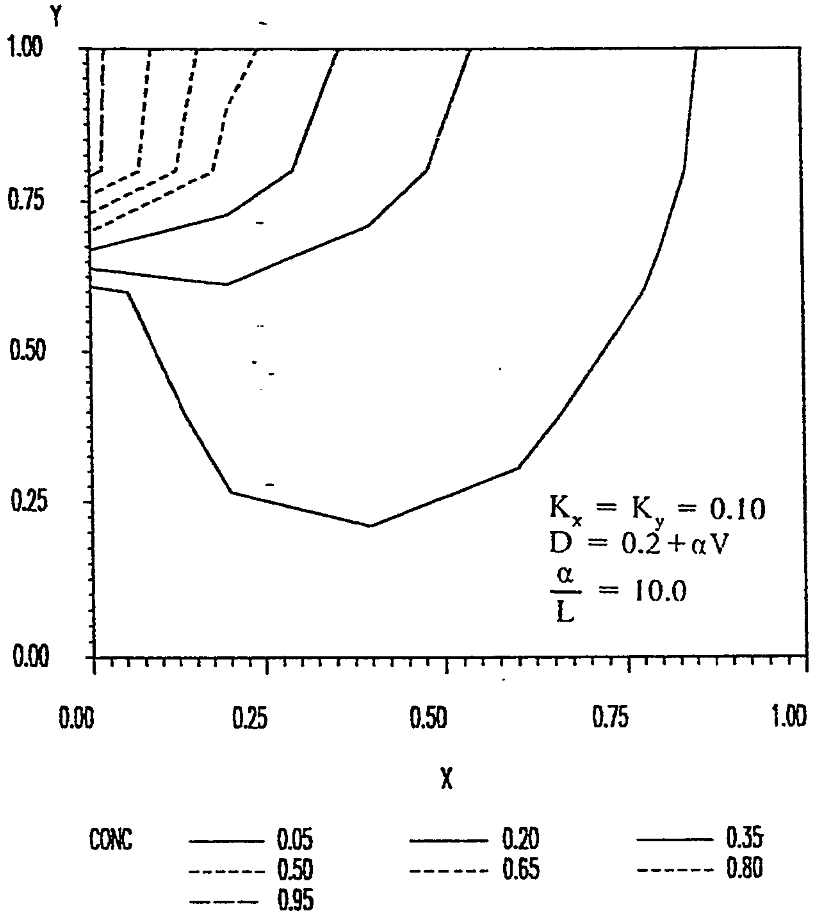
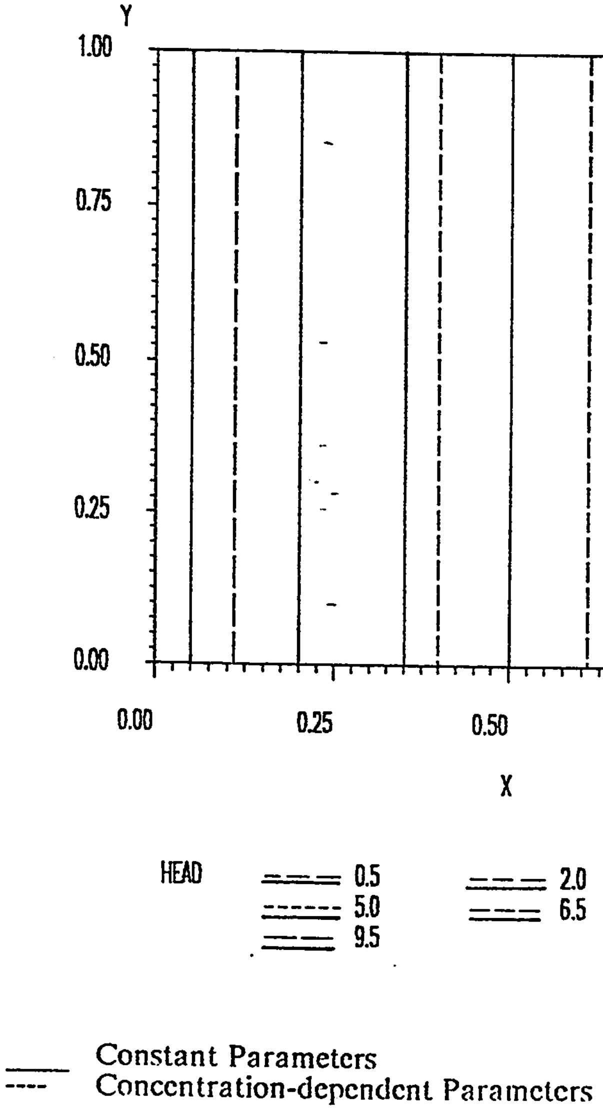


Figure-5.15a: Constant parameter Two-dimensional steady Concentration distribution in two-dimensional space obtained from coupled virtually one-dimensional steady flow field

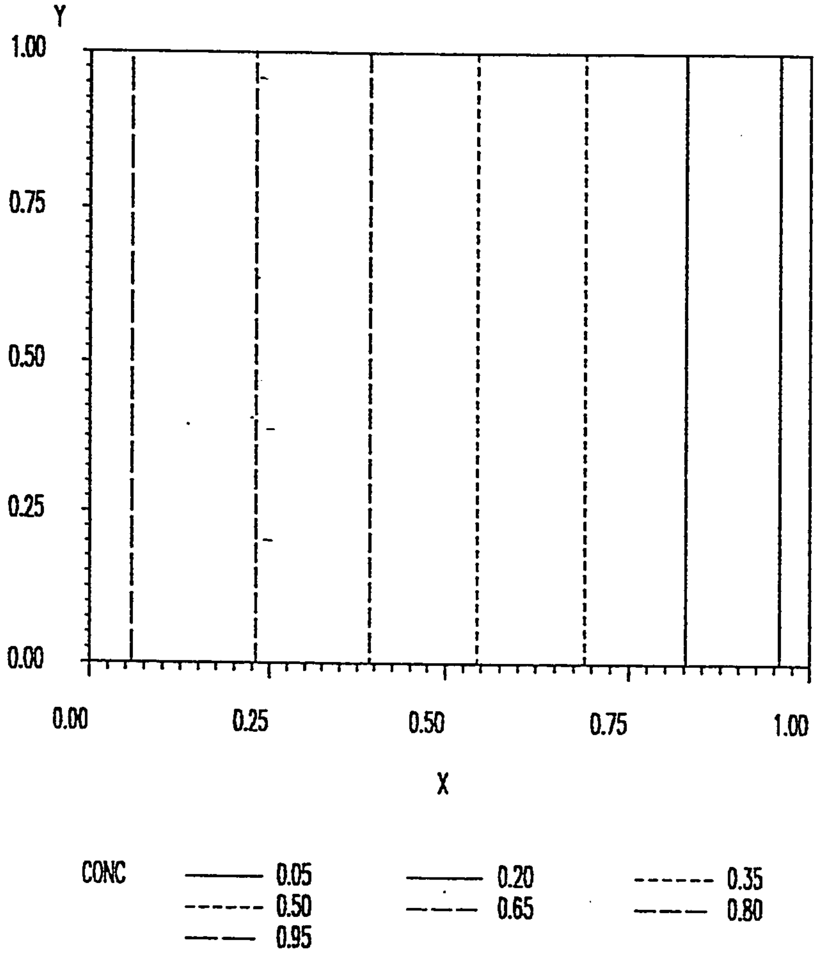


$$\frac{K_x}{K_0} = \frac{K_y}{K_0} = 1+9C$$

$$D_x = D_y = 0.20+\alpha V$$

$$K_0=0.10 \text{ and } \frac{\alpha}{L} = 2.0$$

Figure-5.15b: Comparison of Steady Two-dimensional Head distribution in two-dimensional space obtained from coupled solution for constant and concentration-dependent parameters



$$\frac{K_x}{K_0} = \frac{K_y}{K_0} = 1+9C$$

$$D_x = D_y = 0.20+\alpha V$$

$$K_0=0.10 \text{ and } \frac{\alpha}{L} = 2.0$$

Figure-5.16a: Steady State Concentration distribution in two-dimensional space obtained from coupled solution for concentration-dependent parameters

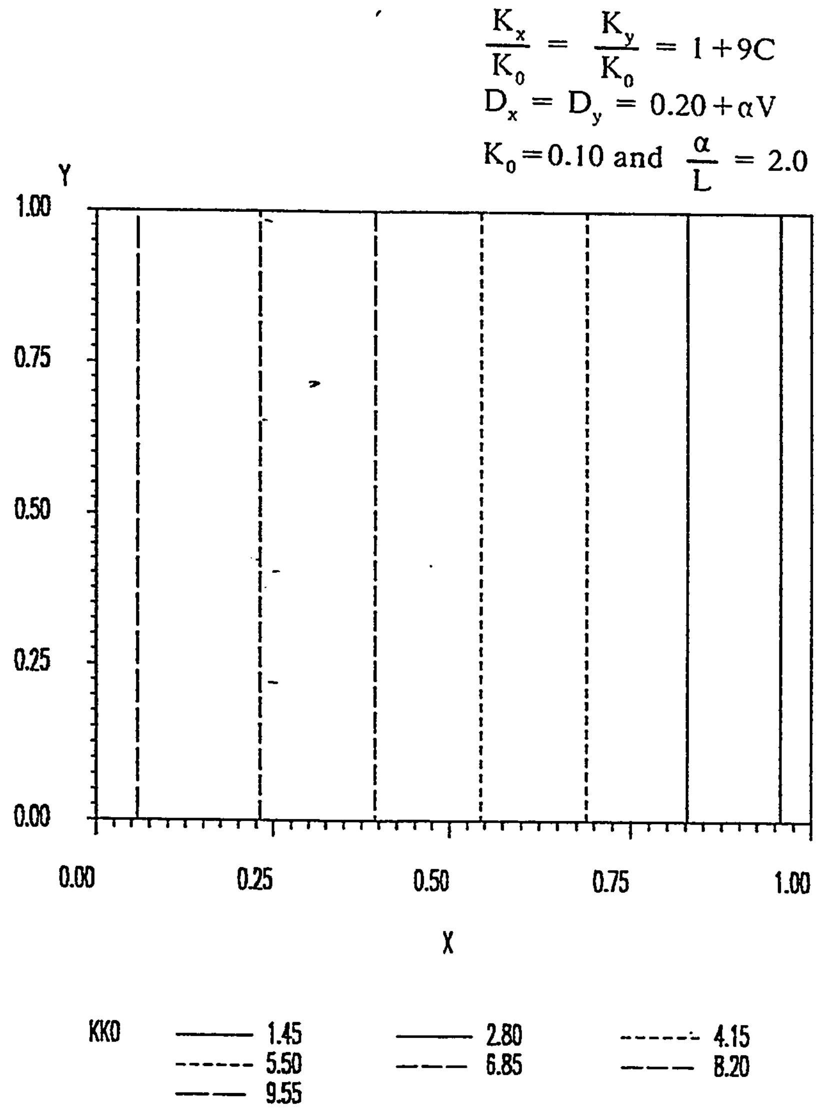


Figure-5.16b: Steady State Hydraulic Conductivity distribution in two-dimensional space obtained from coupled solution for concentration-dependent parameters

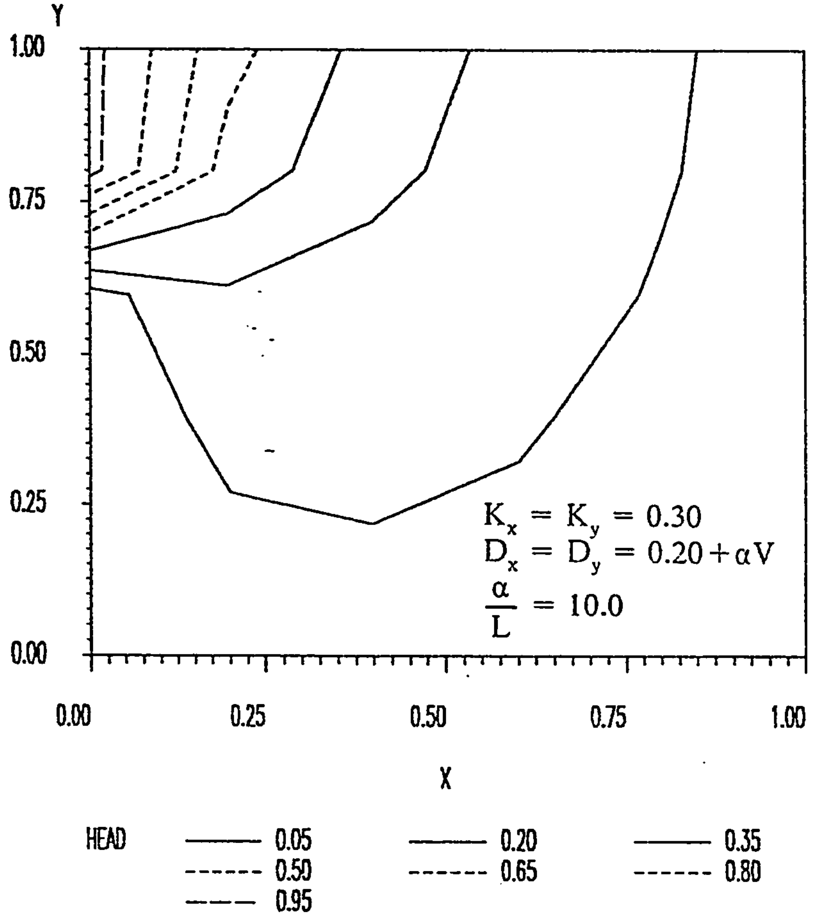


Figure-5.17a: Constant parameter two-dimensional head distribution in two-dimensional flow obtained from coupled solution

$$K_x = K_y = 0.30$$
$$D_x = D_y = 0.20 + \alpha V$$
$$\frac{\alpha}{L} = 10.0$$

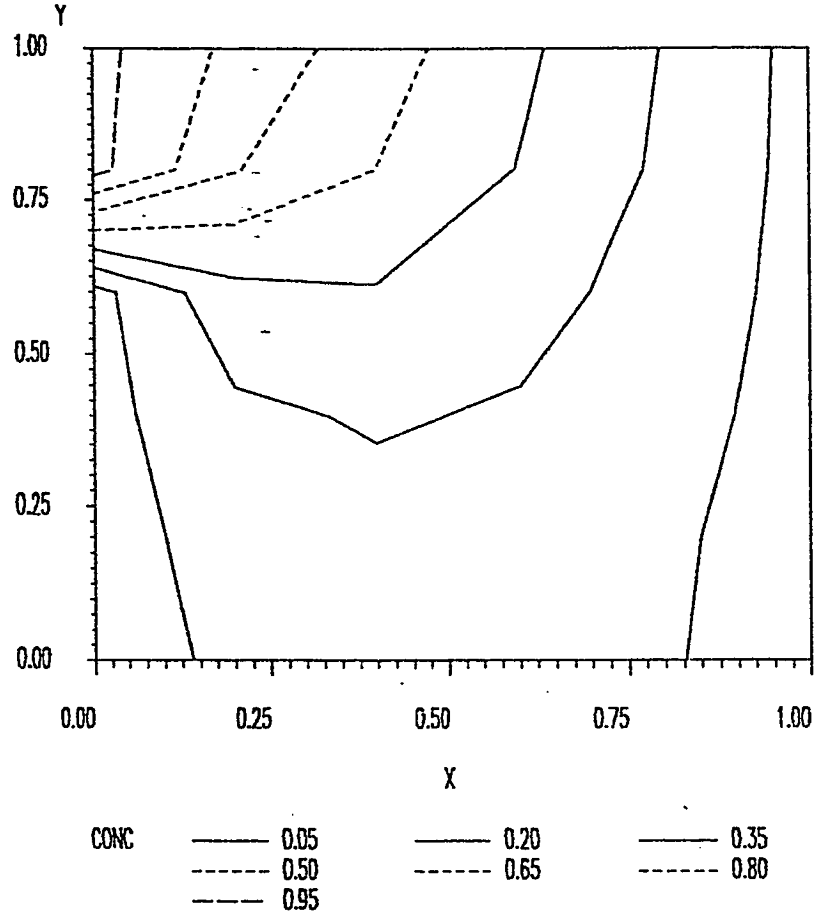


Figure-5.17b: Constant parameter two-dimensional concentration distribution in two-dimensional flow obtained from coupled solution

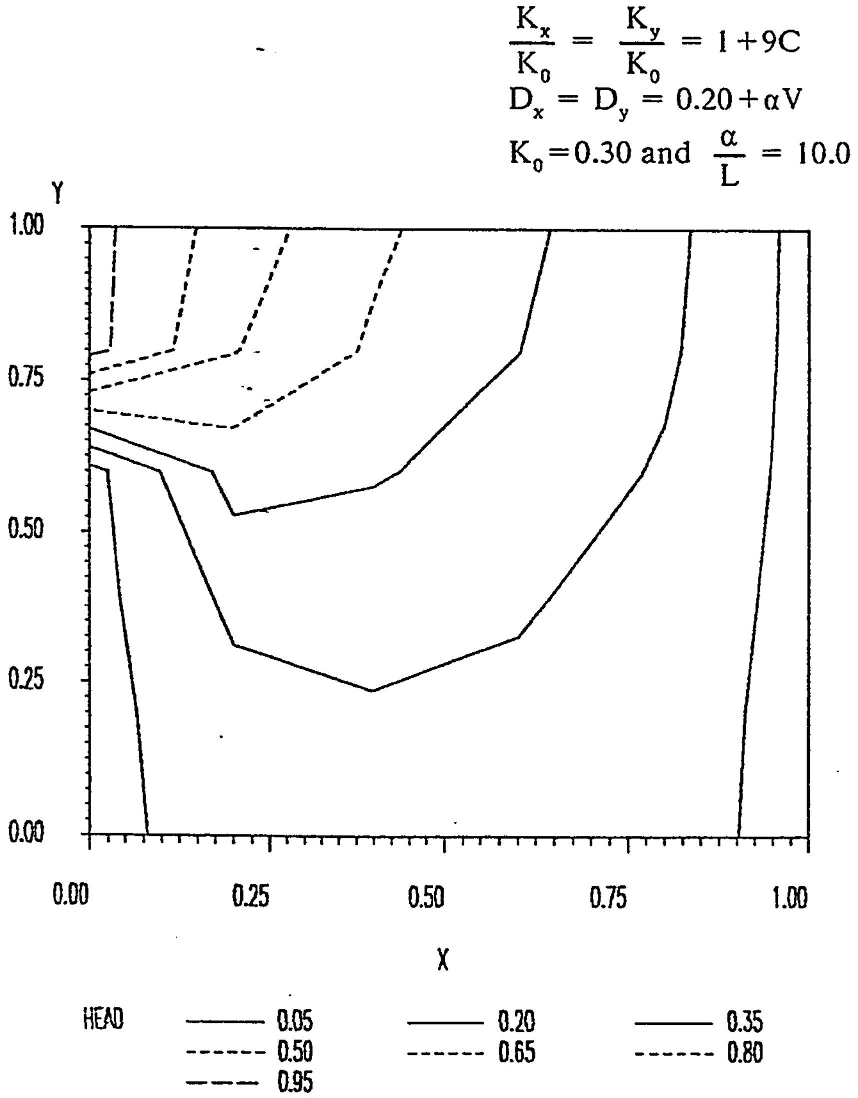


Figure-5.18a: Steady two-dimensional head distribution in two-dimensional flow field obtained from coupled solution for concentration-dependent parameters

$$\frac{K_x}{K_0} = \frac{K_y}{K_0} = 1+9C$$

$$D_x = D_y = 0.20+\alpha V$$

$$K_0=0.30 \text{ and } \frac{\alpha}{L} = 10.0$$

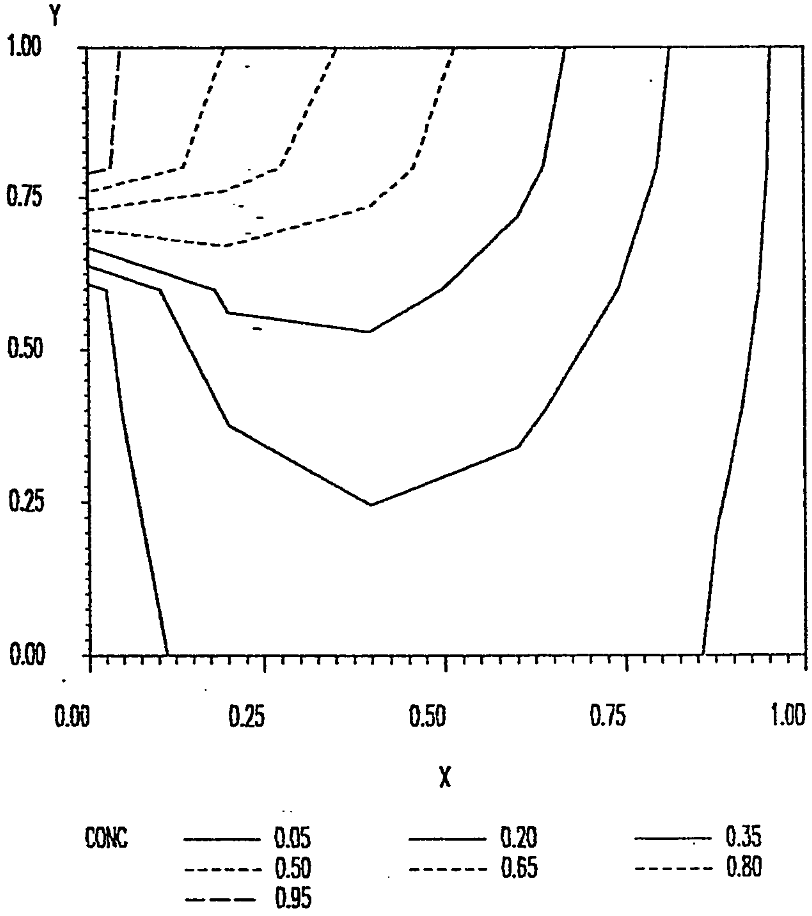


Figure-5.18b: Steady two-dimensional concentration distribution in two-dimensional flow field obtained from coupled solution for concentration dependent parameters

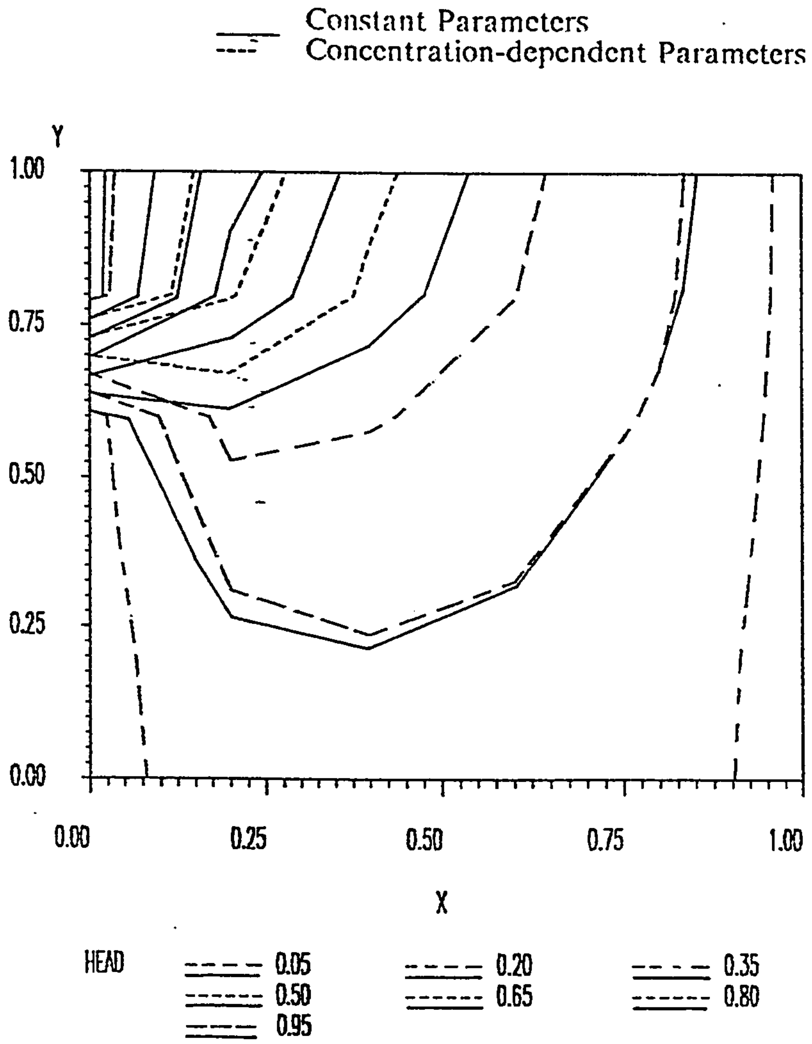


Figure-5.19a: Comparison of Steady two-dimensional head distribution in two-dimensional flow field obtained from coupled solution for constant and concentration-dependent parameters (obtained from figures 5.17a and 5.18a)

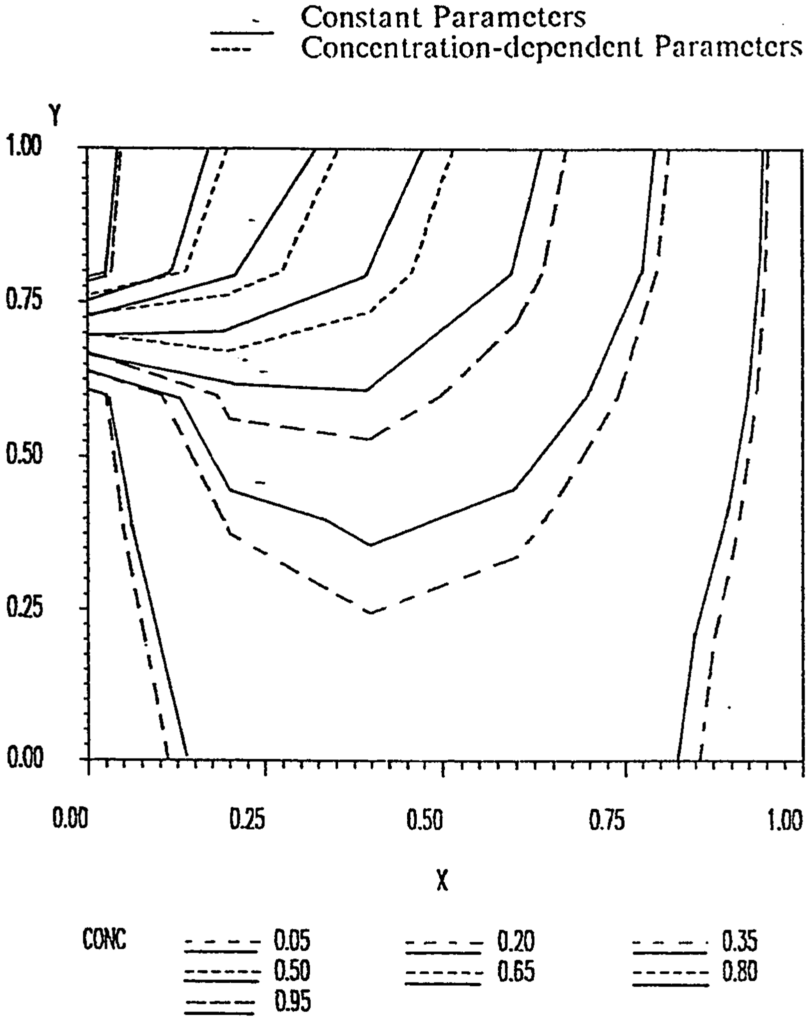


Figure-5.19b: Comparison of Steady two-dimensional concentration distribution in two-dimensional flow field obtained from coupled solution for constant and concentration-dependent parameters (obtained from figures 5.17b and 5.18b)

$$\frac{K_x}{K_0} = \frac{K_y}{K_0} = 1+9C$$

$$D_x = D_y = 0.20+\alpha V$$

$$K_0=0.30 \text{ and } \frac{\alpha}{L} = 10.0$$

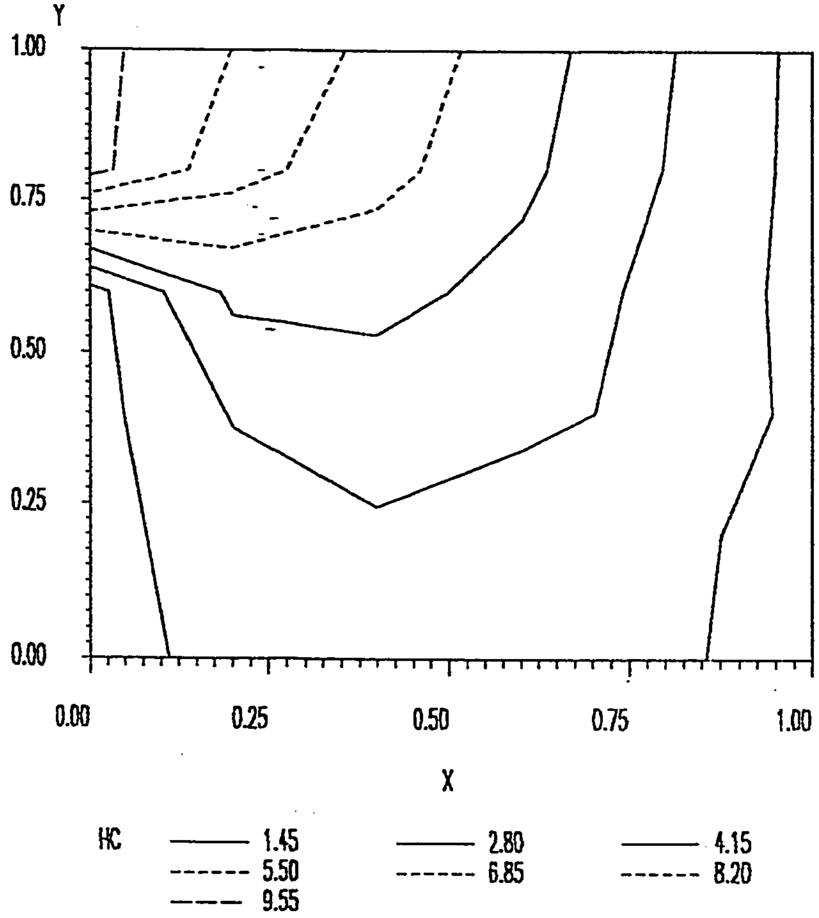


Figure-5.19c: Steady State Hydraulic Conductivity distribution in Two-dimensional flow field obtained from coupled solution for concentration-dependent parameters

$$\frac{K_x}{K_0} = \frac{K_y}{K_0} = 1+9C$$

$$D_x = D_y = 0.20+\alpha V$$

$$K_0=0.30 \text{ and } \frac{\alpha}{L} = 10.0$$

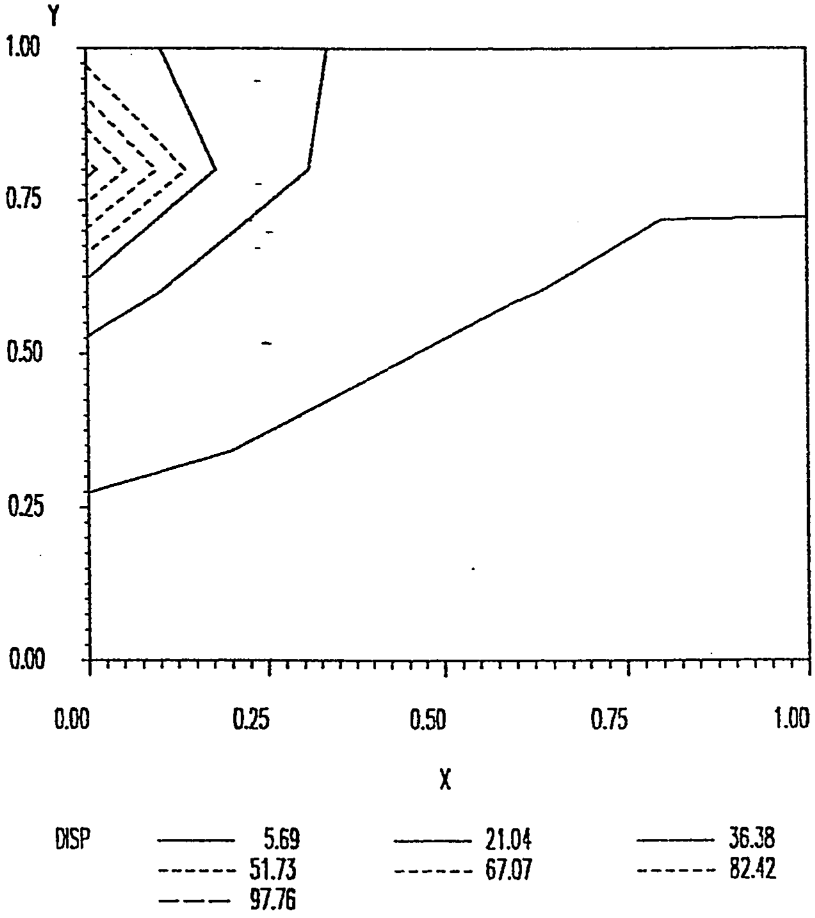


Figure-5.19d: Steady State Dispersion Coefficient distribution in Two-dimensional flow field obtained from coupled solution for concentration-dependent parameters.

5.4 RESULTS AND DISCUSSIONS

The computer code is found to produce very satisfactory results for a variety of test problems. The results are presented in the earlier sections.

The magnitude of the rate of change of porosity term in the solute aggressiveness factor has larger value at the initial stage of the transient problem and decreases gradually as the system approaches steady state.

The effect of the solute aggressiveness factor ultimately becomes an induced heterogeneity factor as the steady state condition is reached for the transport equation, leaving a completely different heterogeneous medium.

When the concentration-dependent model parameters are considered (figure-5.6d and figure-5.8d, i.e. aggressive solutes), the incompressible unsteady flow exists as long as the transport equation remains transient, irrespective of the rate of change of porosity in the solute aggressiveness factor.

The distribution of steady state variables is the same for concentration dependent parameters and the aggressive case, since the transient part of the aggressiveness factors exists only during the transient state.

The medium characteristics satisfying the Kozeny-Carmen equation , which relates the intrinsic permeability to the effective porosity, needs to be investigated considering the aggressiveness factor.

When the medium intrinsic permeability is related to effective particle diameter, the coupled system needs to be solved simultaneously considering the concentration-dependent parameters when appropriate.

The simultaneous solution of the system of equations for concentration dependent model parameters yields

i) a heterogeneous medium when the medium is initially homogeneous

ii) a medium with increased heterogeneity since the aggressive solutes introduces additional heterogeneity.

iii) a homogeneous medium with completely different medium properties when the steady state concentration distribution is uniform (depending on downstream boundary conditions and/or the magnitude of the model parameters).

The numerical results also demonstrated that the significance of the solute aggressiveness phenomena depends on the degree of aggressiveness exhibited by the permeant. The solute aggressiveness factor is a time-dependent parameter which complicates the transient solution procedure of the governing equations. A comparative study indicated significant differences in the predicted values at the earlier stage due to the above mentioned reasons. The differences, however, decreases with time (figures-5.11c-11i). The induced heterogeneity in model parameters was appeared to be important. The transient behavior of the dependent variables also suggested the insignificance of time variance of porosity for long term transient problems.

5.5 SALIENT FEATURES OF THE MODEL

1. The proposed model is developed emphasizing the need of simultaneous solution of the groundwater flow and transport equations since these two processes are coupled in the natural system.

2. A very few models have been reported and most of them are developed for the concentration-independent model parameters. A variety of concentration dependent model parameter is considered here.

3. The majority of the existing models consider only linear systems with respect to model parameters, but in this study, a nonlinear system is derived from the basic concept for aggressive solutes.

4. The solution techniques used in the available models are the finite difference schemes which gives step function type discontinuous velocity field, not conformable to heterogeneous medium and/ or variable parameter problems. In the present work, a continuous velocity field is guaranteed by using higher order polynomials and more than one degree of freedom per node.

5. The algorithm used avoids numerical differentiation which inherent uncertainty and difficulties. It is avoided imposing C^1 continuity condition in the collocation finite element formulation.

6. The developed model is capable of dealing with any type of medium

heterogeneity

7. It provides eleven different options for the user as explained in Appendix-D.

8. Nonlinear variations of the medium properties as well as the model parameters were considered using the cubic hermitian interpolation functions.

9. The pseoudonormalized form of the equations guaranteed the same real time corresponding to the normalized time for the both equations and also provided additional computational advantage.

10. Only the controlling parameters are required to be changed to solve different problems.

11. Data input is made to be possible minimum since the grid is generated automatically inside the main programme (Appendix-E).

12. It is capable of handling different type of boundary and initial conditions for the two governing differential conditions

13. In case of concentration-dependent model parameters, only the respective functional relationship is required to be modified.

14. Steady state results can be obtained directly using minimum computational efforts.

5.6 LIMITATIONS OF THE THEORETICAL DEVELOPMENT

1. The experimental verification needs sophisticated set ups and long time observation since uncertainty is the inherent problem in the study of any phenomena in porous media.

2. Since no study has been reported in the literature describing the solute aggressiveness phenomena, only the significance of the process can be evaluated by numerical experiments.

3. This formulation is not directly applicable to immiscible and/or multi-phase flow and transport. However, similar type of formulation would be possible for such cases.

4. Any change in the microscopic level is not considered in the formulation since it is carried out at macroscopic level as is the usual practice.

5. If extensive studies on different phenomena suggests the significance of any change in the microscopic level , microscopic formulation, would yield better representation of the system.

6. The use of the proposed formulation may be considered as the approximation of the lumped microscopic changes interms of macroscopic variables.

7. If the interactions between the various factors results with no change in porosity, the governing equations reduces to the conventional equations, but the existence of concentration-dependent permeability

strongly suggests the need for simultaneous solution of the two governing equations along with the additional equations. It also indicates the existence of unsteady incompressible flow condition as the head distribution in this case is transient.

8. The applicability of the proposed formulation depends on the predominant aggressive mechanism involved.

9. Evaluation of the effect and/or the significance of this phenomena would decide the span of application of the proposed formulation as well as that of the conventional one.

10. The results of the numerical experiments would also suggest the need and/or the directions of experimentations. A comprehensive numerical experiment might save some experimental effort.

11. The microbial growth kinetics is not incorporated in these model. Recent studies have amply demonstrated the remarkable effect of Microbial growth on flow dynamics and contaminant movement in natural systems (Taylor et.al. (1990a,1990b,1990c,1990d)). Importance of modeling natural system incorporating microbial growth kinetics is also emphasized by Khondaker et.al. (1990).

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Chapter VI

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

The study of solute transport in porous media related to groundwater contamination in particular is in the midst of an exciting period of growth and challenge. A review of literature published during the last two decades has revealed progress in many areas. Investigators have uncovered a number of inadequacies with our existing scientific understanding of subsurface transport models, furthermore, they have made significant strides toward achieving a better understanding of these important phenomena.

Some new research areas such as biodegration modeling, transport in fractured media, immiscible transport, solute effects on medium properties, and inverse techniques for the optimal estimation of the model parameters, are just emerging. Researchers from a wide variety of disciplines have been involved in these investigations.

As this literature review amply demonstrates, the advancements in scientific understanding of the variety of processes which affect the transport and persistance of contaminants in the subsurface environment illustrate the complexity of the subsurface transport processes. Proper treatment of this complexity demands increasing specialization in the area of groundwater contamination studies.

Indeed, no individual can claim to have an in-depth understanding of all phenomena. Enormous growth has occurred during the last two decades in experimental, analytical, and numerical modeling directed toward a large array of problems. These are reported in an overwhelming number of journals from different disciplines. The necessity of interdisciplinary cooperation among investigators is essential for the future advancements in our ability to deal with groundwater contamination problems.

Another general observation to be gleaned from this review is that investigators in a variety of disciplines have come to the realization that controlled field experimentation is necessary for the verification, future development and calibration of modeling approaches.

The objective of the present work is two-fold, namely;

a) a systematic review and critical analyses of the developments of research in this area to summarize the research trends and the associated forthcoming challenges

b) Modeling of the coupled process of groundwater flow and solute transport emphasizing on the effects of solute aggressiveness on the fundamental properties of porous media.

The salient features of the present work is summarized below:

1. An extensive literature survey furnished the idea of the present status of the research activities in the broad spectrum of groundwater contamination.

2. The unresolved problems are identified for future research and the potential directions are indicated

3. An inventory of the available models is presented

4. Solute aggressiveness phenomena is identified as one of the important aspects of flow and transport modeling in porous media and investigated theoretically.

5. A mathematical representation of solute aggressiveness phenomena is proposed.

6. A modified system of nonlinear equations governing the flow and transport of the aggressive solutes are derived .

7. A solution algorithm is proposed to solve the system of nonlinear equations simultaneously.

8. A numerical model is developed implementing the proposed algorithm using advanced technique of collocation finite element.

9. The developed numerical model is capable of solving the natural coupled system of flow and transport in porous media for different combinations

The following conclusions can be made from the numerical studies.

a) Solute aggressiveness phenomena changes the medium properties introducing additional heterogeneity, which is considered to be a major cause of uncertainty and failure in achieving any reliable relationship between the field and the laboratory values of the model parameters.

b) Induced heterogeneity appears to be significant

c) As the solute movement remains transient, groundwater flow remains transient as well.

d) Incompressible, unsteady flow condition exists because of heterogeneity that is induced by the time dependency of the model parameters

e) The effect of heterogeneity due to the change in medium porosity is larger at the earlier stage and insignificant at the latter stage.

f) The significance of the overall effect of solute aggressiveness depends on the degree of aggressiveness exhibited by the permeant.

g) The effect of solute aggressiveness on solute movement pattern depends on the extent of change in Peclet number.

h) In long term transient problems, the effect of intrinsic permeability expression appears to be insignificant.

i) The existence of solute aggressiveness phenomena requires simultaneous solution of the governing equations.

RECOMMENDATIONS

The study of solute aggressiveness phenomena, being a new frontier, needs further comprehensive investigation. The primary effect of solute aggressiveness is the introduction of heterogeneity in the medium. The variations in medium properties like hydraulic conductivity and porosity certainly affects the flow dynamics and the movement of chemicals as well through the porous media.

The mathematical model proposed here considered an idealized and conceptual porous medium, obviously quite different from the natural system. The natural system contains organic materials and various minerals. Furthermore, there may be biological reactions because of the presence of organic matters and the microorganisms in the natural system. The experimental study has amply demonstrated the remarkable effects of microbial growth on the flow dynamics and the movement of contaminants in the porous media. Recent studies reported a 5,000 times reduction in hydraulic conductivity in sand columns. One way to deal with the problem of microbial growth in the natural system and/or the movement of organic chemicals in the subsurface environment is to incorporate the microbial growth kinetics in the development of the mathematical models for the systems.

The variations of the model parameters considered here were based on the study of idealized laboratory systems. The comprehensive experimental investigations should be made in the field of a representative size. From the tracer tests in the field, one can evaluate the instantaneous velocity and the effective porosity simultaneously. Determination of effective porosity and its variations due to solute nature and/or concentration, would certainly provide a better understanding of the solute aggressive phenomena.

The flow encountered in the natural system is rarely saturated, and the medium considered could be anisotropic. The unsaturated flow and/or the medium anisotropy makes the problem much more complicated. However, all these factors are needed to be studied in order to understand the physical phenomena properly and to predict the flow dynamics and the movement of chemicals in the natural systems accurately and effectively.

Simulation models are not truly predictive tools in a classic scientific sense. The use of mathematical models to simulate the behavior of any complex natural system lies somewhere between science and art. The study of such natural systems is a never-ending activity and improvements are continuously being made as more understanding and information become available.

APPENDIX - A1

Inventory of Solute Transport Models

APPENDIX - A1 : Inventory of Solute Transport Models

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Ahlstrom et.al.,1974				X		X			X		X			X	X	
Al-Niami and Rushton,1977									X							
Anand and Pandit,1982										X					X	
Andersen et al.,1986	X									X						
Andersen et al.,1988										X			X			
Angelakis et al.,1987	X			X		X		X	X					X		
Babu and Pinder,1984				X		X	X			X						
Baetsle,1967	X			X		X	X									
Barnes,1986	X			X		X	X		X					X	X	X
Basak and Murty,1978									X							
Bear,1972	X			X	X	X	X	X	X					X	X	X
Bird,et al.,1960	X			X	X	X	X	X	X					X		
Boast,1973			X	X	X	X	X									
Boochs and Barovic,1981			X	X	X	X	X							X		
Bower,et al.,1957				X	X		X		X			X			X	
Bredehoeft and Pinder,1973										X					X	
Bresler and Laufer,1974				X		X				X		X			X	
Bruch et al.,1967	X								X						X	
Cameron and Klute,1977				X	X	X			X			X			X	
Carnahan, 1975	X															
Carnahan, 1976	X															
Carnahan,et al., 1984				X			X	X		X			X		X	
Cassel, et al., 1975				X			X	X		X			X		X	X
Cederberg, et al., 1985	X		X		X	X	X		X		X	X		X		
Charbeneau, 1981				X			X	X	X					X		
Charbeneau,1982	X			X		X	X		X					X		
Charbeneau,1984	X			X		X	X		X					X		X
Chu and Sposito,1981	X			X	X											
Cleary and Ungs,1978									X							
Coats and Smith,1964			X						X			X			X	
Colwell and Dranoff,1969					X	X	X			X				X		
Corey et al.,1976				X	X	X			X				X		X	X
Crittenden and Weber, 1978a					X		X			X		X			X	
Crittenden and Weber, 1978b					X		X			X		X			X	
Crittenden and Weber, 1978c					X		X			X		X			X	
Crittenden et al,1986	X			X	X	X	X			X				X	X	
Corwin and Farmer,1984				X			X		X		X					

Contd.

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Dagan ,1984	X															
Dagan ,1988	X									X						
Davidson, et al,1975				X			X			X		X			X	X
Davidson et al.,1986	X			X		X			X							
De Smedt and Wierenga, 1979			X			X			X					X		
De Smedt and Wierenga, 1984			X						X						X	X
Domenico, 1977	X			X	X	X	X	X								
Dudley, et alc, 1981		X		X			X	X		X			X			X
Duffy, et al, 1975				X	X	X	X			X			X		X	X
Dutt, et al, 1972		X		X			X	X		X	X	X	X		X	
Elzeftawy, et al., 1976				X		X				X		X			X	X
Enfield and Shew, 1975				X	X				X	X		X			X	
Enfield, et al., 1976					X	X	X		X		X					
Enfield,et al.,1986	X		X			X			X							
Enfield, et al., 1981a					X	X				X	X					
Enfield, et al., 1981b					X	X	X			X			X		X	
Ferrel, et al., 1976					X		X		X			X			X	
Fried, et al., 1977				X		X			X							
Frind,1982										X					X	
Fungeroli and Steiner,1979				X		X				X			X		X	X
Galya, 1987	X			X		X			X							
Gaudet, 1977			X									X				X
Glas and McWhorter, 1976		X		X			X			X		X				
Goldstein, 1953a	X			X	X	X	X		X							
Goldstein, 1953b	X			X	X	X	X		X							
Grenny et al.,1987	X		X	X		X	X			X		X				X
Griffin and Jurinak, 1973					X		X			X	X					
Grove, 1976				X	X	X	X									
Grove, 1977				X		X										
Grove and Rubin, 1976				X	X	X				X			X			
Grove and Stollenwerk, 1984				X		X	X			X				X		
Grove and Stollenwerk, 1985					X		X									
Grove and Wood, 1979		X		X			X	X		X	X	X	X		X	
Gureghian, et al., 1979					X	X	X		X		X					X
Guven and Molz,1986	X								X							
Harter, 1976		X		X		X				X	x			X		
Harter, 1984				X							x					
Hassanizadeh,1986	X		X					X								
Hassanizadeh,1986a	X		X	X				X								

Contd..

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Hassanizadeh and Leijnse,1988	X									X						
Hassanizadeh and Gray, 1979	X			X	X	X										
Heinrich and Yu,1987										X						
Helfferich, 1962		X			X	X	X			X						
Hiester, et al., 1956					X		X				X				X	
Hill and Lake, 1978				X		X	X	X				X			X	
Huggenberger, et al., 1972				X	X	X	X			X	X	X				
Hunt,1978										X					X	
Hutzler, et al., 1986			X	X	X	X			X		X			X		
Huyakorn et al.,1986						X				X					X	
Huyakorn and Taylor,1976										X					X	
Jackson and Inch, 1983				X		X			X		X		X	X		
James and Rubin, 1979				X	X	X				X		X			X	
Jardine and Sparks, 1984					X		X				X					
Jennings, et al., 1982	X			X			X	X		X				X		
Jennings and Kirkner, 1984				X	X		X	X		X				X		
Jurinak, et al., 1974		X		X	X		X	X				X			X	
Jury,et al., 1986a				X		X			X		X	X	X			X
Jury,et al., 1986b	X															
Kay and Elrick, 1967				X		X			X			X			X	
Kim, et al., 1978	X				X		X			X	X	X			X	
Kipp, et al., 1986				X		X	X	X					X		X	
Kirkner, et al., 1984	X	X	X	X	X											
Kirkner, ey al., 1985				X	X		X	X		X		X			X	
Kreft and Zuber,1978	X								X							
Krupp and Elrick, 1968			X									X				X
Kumer, 1983				X		X			X					X		
Lai and Jurinak, 1971				X		X	X			X		X			X	
Lake and Helfferich, 1978				X			X	X		X				X	X	
Lapidus and Amundson, 1952				X	X	X	X		X					X		
Laryea, et al., 1982				X			X			X		X				
Lassey,1988	X		X	X		X			X							
Leistra, 1977				X		X				X				X		
Lin, 1977				X			X			X				X		
Lin, et al., 1983a					X					X	X					
Lin, et al., 1983b					X					X		X			X	
Lindstrom and Boersma, 1970				X		X	X			X				X		
Lindstrom and Boersma, 1971					X		X		X					X		
Lindstrom et al.,1967	X			X		X			X							

Contd.

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Lindstrom and Narashimhan,1973	X			X		X			X							
Lund, et al., 1975				X	X	X	X		X			X			X	
Mansell, et al., 1977					X		X				X	X			X	X
Marino, 1974a				X		X			X					X		
Marino, 1974b				X		X			X					X		
Marino, 1978				X		X			X					X		
Mauersberger, 1978	X			X	X	X	X									
Mehnert and Jennings,1985			X							X				X		
Melamed, et al., 1977				X	X	X	X		X	X		X			X	
Mercado, 1977					X		X			X			X		X	
Metry, 1976				X	X	X	X			X				X		
Miller and Benson, 1983				X			X	X		X				X		
Miller and Weber,1988				X		X					X					
Mohsen and Baluch,1983									X						X	
Murali and Aylmore, 1983				X			X	X		X				X		
Nguyen, el al. 1982					X		X	X						X		
Nielsen and Bigger, 1961				X		X			X			X				
Neilsen, et al., 1986			X	X	X	X	X									X
Nkedi-Kizza, et al., 1982			X	X			X			X	X	X			X	
Nkedi-Kizza, et al., 1984	X		X	X	X		X			X		X			X	
Novak, et al., 1975					X		X		X		X					
Novak and Adriano, 1975					X					X			X			
Oddson, et al.,1970	X			X		X			X							
Ostendorf, 1986				X	X	X			X				X		X	
Ostendorf, et al., 1984		X		X	X	X			X							
Parker and Jardine, 1986				X	X					X		X		X	X	
Parker and Valocchi, 1986				X	X	X	X		X					X	X	
Parker,et al,1986	X		X							X						X
Parlange and Starr, 1978					X	X			X					X		
Persuad and Wierenga, 1982	X			X			X			X		X			X	X
Pickens, et al., 1979				X		X			X					X		
Pickens and Lennox, 1976			X		X					X				X		
Pickens, et al., 1981				X		X				X	X	X	X		X	
Pinder,1984	X															
Pope, et al., 1978	X			X			X	X								
Prakash, 1976				X	X	X	X			X				X		
Price et.al.,1968										X						
Rachinskii, 1978	X			X	X	X	X		X							
Rao, et al., 1979			X	X	X	X	X			X			X			X

Contd.

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Rao, et al., 1980a			X							X		X				
Rao, et al., 1980b			X							X			X			X
Reardon, 1981		X		X		X										
Reeves, et al., 1977				X		X		X		X				X		
Robertson, 1974				X	X	X				X			X			
Robertson, 1977					X	X				X			X	X		
Robertson, et al., 1973				X	X	X				X			X			
Rolston and Marino, 1976					X				X	X		X				X
Routson and Serne, 1972		X		X	X	X	X	X		X		X				
Rowe and Booker, 1985				X		X								X		
Rowe and Booker,1986	X			X		X			X						X	
Rubin, 1983	X			X	X	X	X	X								
Rubin and James, 1973	X			X			X	X		X				X		
Russo, 1988	X									X					X	X
Russo, 1988a	X									X					X	X
Russo, 1986																
Said, 1956		X		X		X			X					X		
Saxton, et al.. 1977		X		X				X		X			X			X
Schulin et al.,1987													X			
Schulin et al.,1987a			X									X				X
Schultz and Reardon, 1983		X		X			X	X		X			X	X	X	
Schwartz and Dominico, 1973				X	X	X				X				X		
Schartz, 1975				X	X	X	X	X		X			X			
Schwartz et al.,1987		X		X			X	X		X						X
Schweich and Sardin, 1981	X			X	X	X	X	X								
Selim, et al., 1977				X	X	X	X			X	X				X	X
Selim and Manshell,1976				X		X			X			X				
Serne, et al., 1973		X		X			X	X		X	X	X				
Shaffer and Dutt, 1973		X		X	X		X	X		X	X					
Shah,et al. 1975					X		X			X		X			X	
Shen ,1976				X		X			X						X	
Sposito,et al.1986						X		X	X	X					X	
Srinivasan and Mercer,1988				X		X		X		X						
Sudicky and Frind,1984				X	X	X			X					X		
Symons et al,1988			X	X		X	X			X	X	X				X
Tagamets,1973					X		X			X		X			X	
Tang and Babu,1979										X						
Tanji,1970		X		X			X			X		X			X	

Contd.

Reference	Equation			Chemistry					Solution		Studies					
	TH	MS	MI	EQ	NEQ	LIN	NLN	MSP	ANA	NUM	BAT	COL	FLD	SYN	SAT	USAT
Thomas,et al.,1972		X		X			X	X		X			X			
Travis and Etnier,1981				X	X	X	X									
Valocchi,1984	X			X	X	X				X						
Valocchi,1985	X			X	X									X		
Valocchi,1986																
Valocchi and Roberts,1983				X		X			X					X		
Valocchi,et al.,1981				X			X	X		X			X	X	X	
Valocchi,et al.,1987				X		X			X	X						
van Beek and Pal,1978		X		X			X	X		X		X			X	
van der Zee et al.,1987				X		X										
van Eijkeren and Loch,1984				X			X	X		X		X			X	
van Genuchten and Alves,1982									X							
van Genuchten,et al.,1974				X	X	X	X			X		X			X	
van Genuchten,et al.,1984			X	X		X			X							
van Genuchten and Wierenga,1976			X	X	X		X		X					X	X	
van Genuchten and Wierenga,1977			X						X			X			X	
van Ommen,1985		X		X				X				X	X			
Veith and Sposito,1977	X			X			X									
Vermeulen,et al.1984	X			X	X	X	X									
Vilker and Burge,1979					X	X	X		X		X	X			X	
Walter,et al,1975					X	X	X		X				X			
Weber,1984				X	X	X	X			X				X		
Weber and Miller,1988				X		X						X				
White,et.al.,1986									X			X				
Widdowson et al.,1988																
Wierenga,et al.,1975	X		X				X	X		X	X			X		
Yuan (1986)										X					X	

TH = Theory,MS = Multi-step,MI = Mobile/Immobile,EQ = Equilibrium, NEQ = Non-equilibrium,LIN = Linear,NLN = Nonlinear,MSP = Multi-Species, ANA = Analytical,NUM = Numerical,BAT = Batch,COL = Column,FLD = Field, SYN = Synthetic,SAT = Saturated,USAT = Unsaturated

APPENDIX - A2

HYDRAULIC CONDUCTIVITY VARIATIONS WITH SOLUTE CONCENTRATION

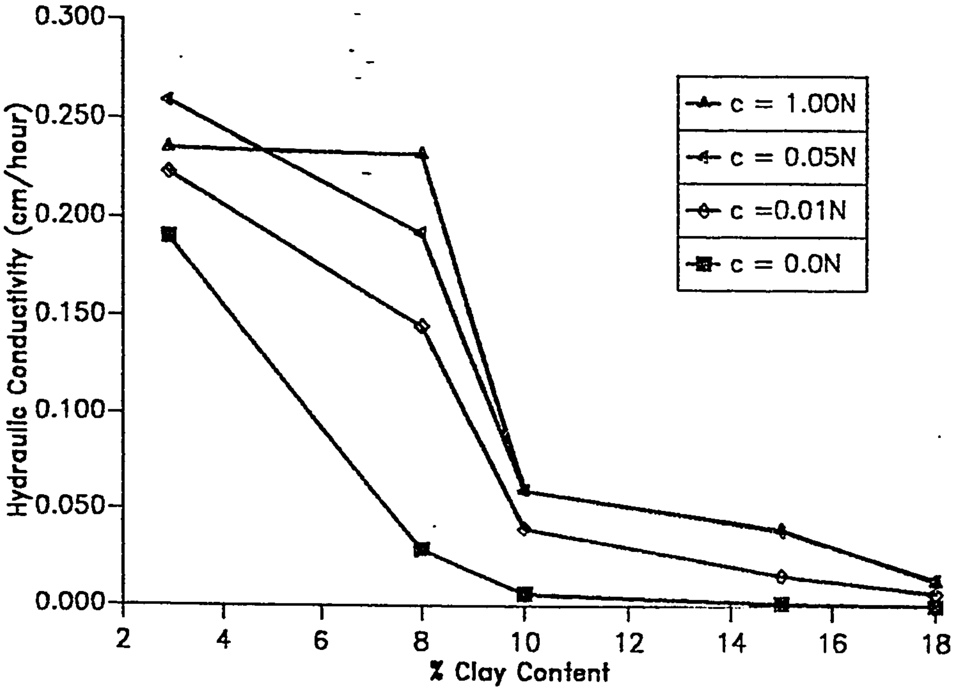


Figure-A2.1: Effect of Clay content and solute concentration on soil Hydraulic conductivity (Frenkel et.al. (1978)).

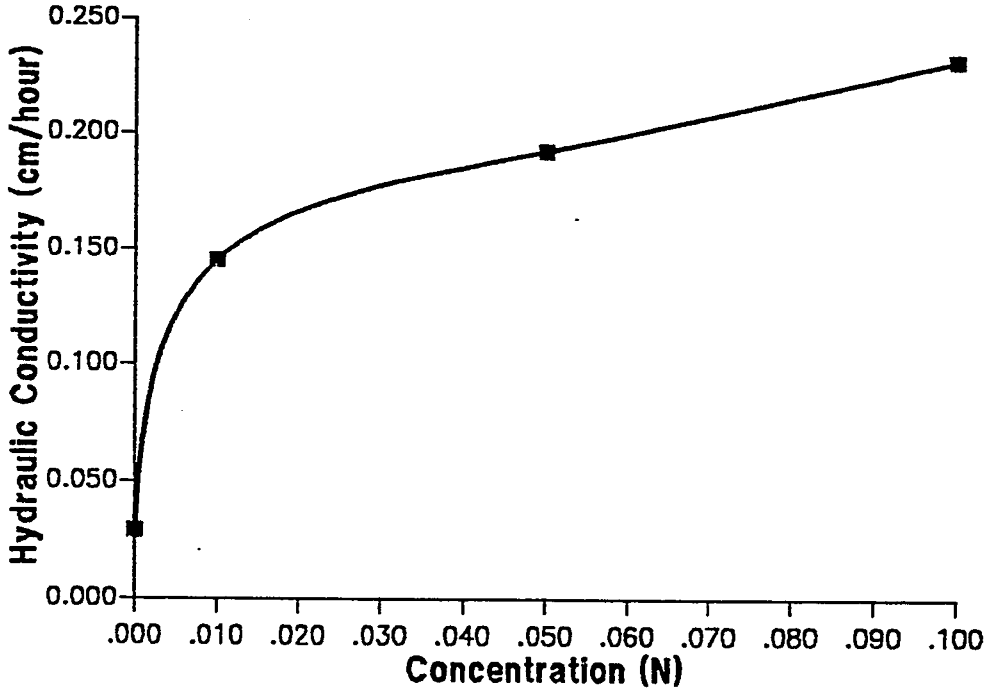


Figure-A2.2a: Effect of solute concentration on soil Hydraulic conductivity for 8% Clay content (Frenkel et.al. (1978)).

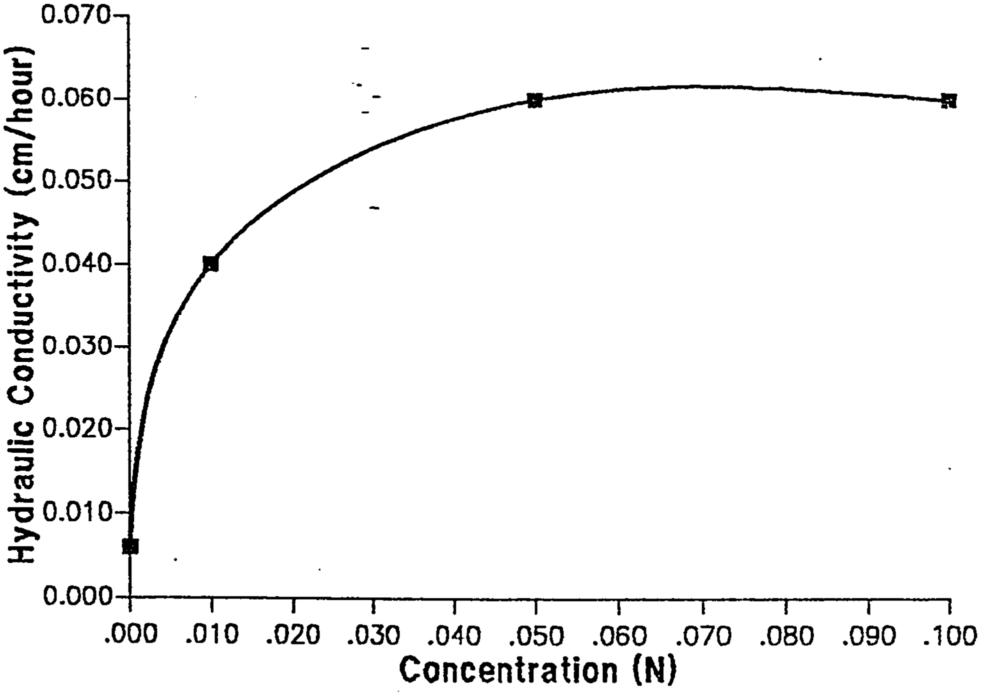


Figure-A2.2b: Effect of solute concentration on soil Hydraulic conductivity for 10% Clay content (Frenkel et.al. (1978)).

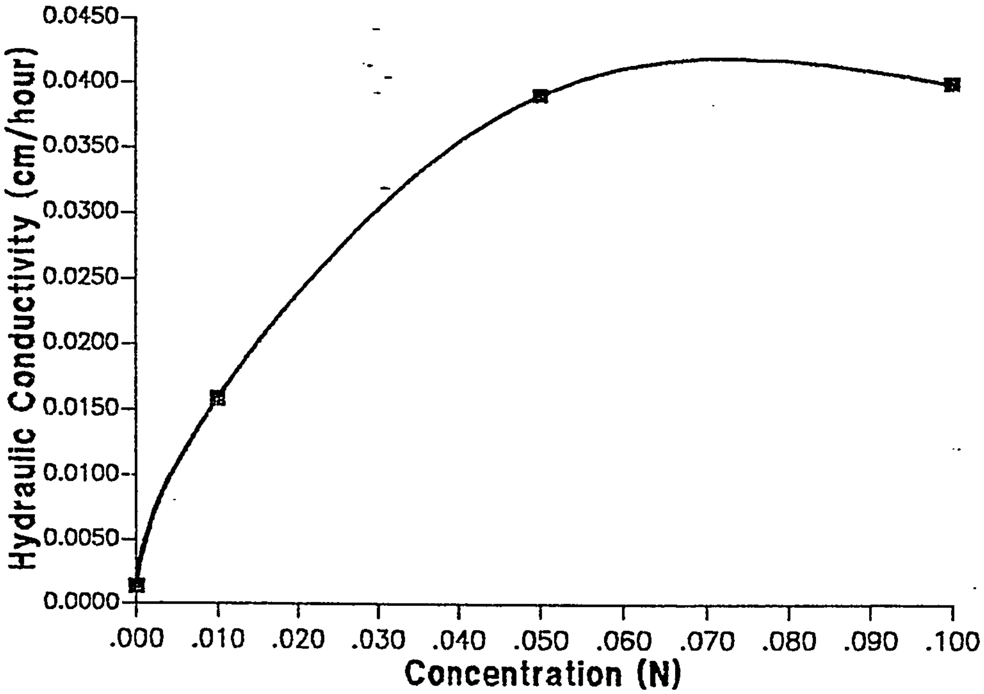


Figure-A2.2c: Effect of solute concentration on soil Hydraulic conductivity for 15% Clay content (Frenkel et.al. (1978)).

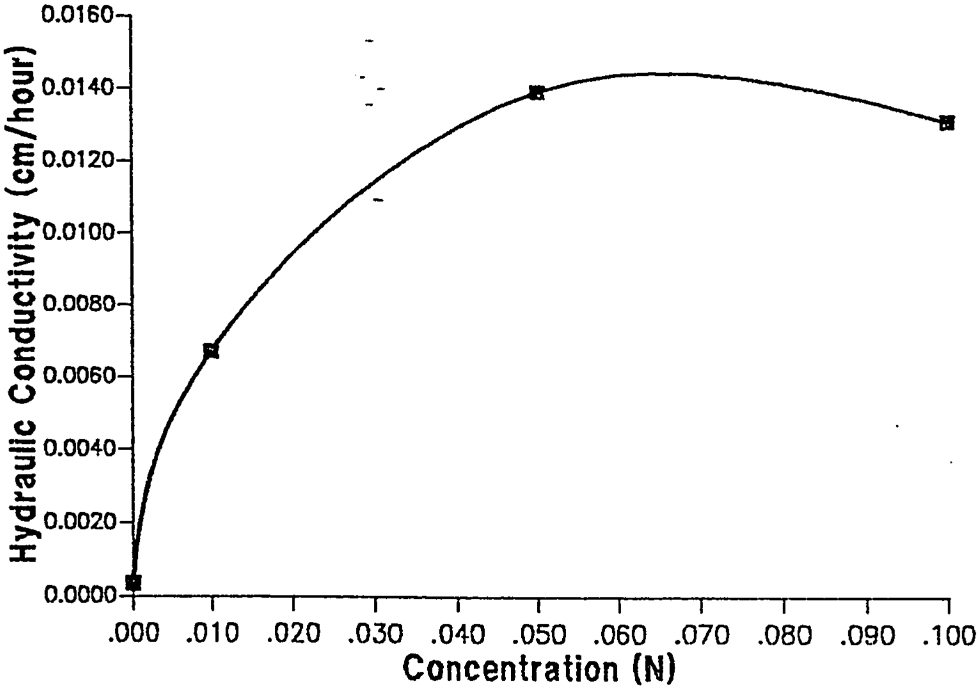


Figure-A2.2d: Effect of solute concentration on soil Hydraulic conductivity for 18% Clay content (Frenkel et.al. (1978)).

APPENDIX - B1

SYSTEM OF GOVERNING EQUATIONS

GOVERNING EQUATIONS AND ADDITIONAL CONDITIONS

I. Groundwater Flow Equation :

$$\frac{\partial}{\partial x_i}(\rho K_{ij}\frac{\partial h}{\partial x_j}) = S\frac{\partial h}{\partial t} + \rho(\frac{\partial \eta}{\partial t})_{s.a.} \qquad (31)$$

II. Boundary Conditions for Flow Equation

III. Initial Conditions for Flow Equation

IV. Transport Equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(Cv_i) - S_a C \qquad (45)$$

V. Boundary Conditions for Transport Equation

VI. Initial Conditions for Transport Equation

VII. Additional Equations.

a) $\rho = f(C)$

b) $\nu = f(C)$

c) $K_{ij} = f(C)$

d) $$\frac{K_t}{K_{t+1}} = \frac{\nu_{t+1}}{\nu_t}(\frac{\eta_t}{\eta_{t+1}})^{3+r}\frac{(1-\eta_{t+1})^2}{(1-\eta_t)^2} \qquad (25)$$

e) $$S_a = \frac{1}{\eta}\{v_i\frac{\partial \eta}{\partial x_i} - \frac{D_{ij}}{C}\frac{\partial C}{\partial x_j}\frac{\partial \eta}{\partial x_i} + \frac{\partial \eta}{\partial t}\} \qquad (43)$$

or $$S_a = \frac{1}{\eta}\{v_i\frac{\partial \eta}{\partial x_i} + \frac{\partial \eta}{\partial t}\} \qquad (44)$$

f) Darcy Equation $v_i = -\frac{K_{ii}}{\eta}\frac{\partial h}{\partial x_i}$

g) $D_i = D_0 + \alpha_i V$

APPENDIX - B2

Newton-Raphson Method

Determination of η_{t+1} from η_t, $\frac{K_{t+1}}{K_t}$ and $\frac{\nu_t}{\nu_{t+1}}$ by Newton-Raphson Method

$$\frac{K_{t+1}}{K_t} = \left(\frac{\nu_t}{\nu_{t+1}}\right)\left(\frac{\eta_{t+1}}{\eta_t}\right)^{3+R} \frac{(1-\eta_t)^2}{(1-\eta_{t+1})^2}$$

Let $X = \frac{K_{t+1}}{K_t}$, $Y = \frac{\eta_{t+1}}{\eta_t}$, $R_n = \frac{\nu_t}{\nu_{t+1}}$ and $A = \frac{1}{\eta_t}$ then,

$$X = R_n Y^{3+R} \frac{(A-1)^2}{(A-Y)^2}$$

$$f(Y) = R^n Y^{3+R}(A-1)^2 - X(A\text{-}Y)^2 = 0 \tag{1}$$

$$\text{And } f'(Y) = R^n(3+R)Y^{2+R}(A-1)^2 + 2X(A\text{-}Y) = 0 \tag{2}$$

The Newton-Raphson iterative scheme for the equations (1) and (2) is

$$Y_{n+1} = Y_n - \frac{f(Y_n)}{f'(Y_n)} \tag{3}$$

APPENDIX - B3

DERIVATION OF EXPRESSION FOR 'S'

DERIVATION OF EXPRESSION FOR 'S'

From the groundwater flow equation (30),

$$\frac{\partial}{\partial t}(\rho\eta)_{def} = [\rho\frac{\partial\eta}{\partial t} + \eta\frac{\partial\rho}{\partial t}]_{def}$$

$$=[\rho\frac{\partial\eta}{\partial p}\frac{\partial p}{\partial t} + \eta\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t}]$$

$$=[\{\rho\frac{\partial\eta}{\partial p} + \eta\frac{\partial\rho}{\partial p}\}\frac{\partial p}{\partial t}] \qquad (I)$$

Defining the coefficient of aquifer compressibility α as

$$\alpha = -\frac{1}{V_b}\frac{\partial V_b}{\partial\sigma}$$

where

$V_b =$ the bulk volume of porous medium

$\sigma =$ is the effective stress

Assuming V_s as the volume of solids in V_b and η as porosity, we have,

$$V_s = (1-\eta)V_b$$

But V_s is constant, therefore

$$\frac{\partial V_s}{\partial\sigma} = (1-\eta)\frac{\partial V_b}{\partial\sigma} - V_b\frac{\partial\eta}{\partial\sigma} = 0$$

Dividing both sides by $(1-\eta)V_b$, we get

$$\frac{1}{V_b}\frac{\partial V_b}{\partial\sigma} = \frac{1}{(1-\eta)}\frac{\partial\eta}{\partial\sigma}$$

But $\alpha = -\frac{1}{V_b}\frac{\partial V_b}{\partial\sigma}$ by definition, therefore ,

$$\alpha = -\frac{1}{(1-\eta)}\frac{\partial\eta}{\partial\sigma}$$

From $\sigma_T = \sigma + p$,we get $d\sigma = -dp$ for constant total stress σ_T due to overburden load. Therefore

$$\alpha = \frac{1}{(1-\eta)}\frac{\partial\eta}{\partial p}$$

which gives

$$\frac{\partial\eta}{\partial p} = \alpha(1-\eta) \tag{a}$$

Defining the coefficient of compressibility of water β as,

$$\beta = -\frac{1}{V_w}\frac{\partial V_w}{\partial p} = \frac{1}{\rho}\frac{\partial\rho}{\partial p}$$

$$\text{or } \frac{\partial\rho}{\partial p} = \beta\rho \tag{b}$$

Substituting (a) and (b) into (I), we get

$$\frac{\partial}{\partial t}(\rho\eta)_{def} = [\rho\alpha(1-\eta) + \beta\eta\rho]\frac{\partial p}{\partial t}$$

$$= \rho[\alpha(1-\eta) + \beta\eta]\frac{\partial p}{\partial t} \tag{c}$$

Now, $p = z+\rho gh$ for plane flow, therefore,

$$\frac{\partial p}{\partial t} = \rho g\frac{\partial h}{\partial t} \tag{d}$$

Substituting (d) into (c), we have

$$\frac{\partial}{\partial t}(\rho\eta)_{def} = \rho^2 g[\alpha(1-\eta) + \beta\eta]\frac{\partial h}{\partial t}$$

Finally, defining $S = \rho^2 g[\alpha(1-\eta) + \beta\eta]$,we obtain

$$\frac{\partial}{\partial t}(\rho\eta)_{def} = S\frac{\partial h}{\partial t}$$

APPENDIX - C

NORMALIZATION OF THE GOVERNING EQUATIONS

INTRODUCTION

The simultaneous solution of the groundwater flow and the solute transport equations require a conformable non-dimensionalization of the variables, since the output of one equation is used in the other one at any time level. It is therefore a necessary condition for non-dimensionalization that it guarrantees the same real time corresponding to the normalized time for both equations. This non-dimensionalized form is obviously different from the widely used ones, where the normalized time expressions contains the model parameters. To assure same real time corresponding to any normalized time for both equations, the normalized time expression is kept independent of model parameters since their values are different. In fact a pseudo-normalized form is used which appeared to be computationally advantageous.

The Governing Equations in Primitive Variables

1. Groundwater Flow Equation

$$\frac{\partial}{\partial X_i}(\hat{K}_{ij}\frac{\partial H}{\partial X_j}) = S\frac{\partial H}{\partial T} + \rho\frac{\partial \eta}{\partial T}$$

Where

$$\hat{K}_{ij} = \rho K_{ij}$$

$$S = \rho^2 g[\alpha(1-\eta)+\eta\beta]$$

Non-dimensionalization

Defining new variables as $x_i = \frac{X_i}{L}$, we have

$$\frac{1}{L^2}\frac{\partial}{\partial x_i}(\hat{K}_{ij}\frac{\partial H}{\partial x_j}) = S\frac{\partial H}{\partial T} + \rho\frac{\partial \eta}{\partial T}$$

Multiplying by L^2, it follows

$$\frac{\partial}{\partial x_i}(\hat{K}_{ij}\frac{\partial H}{\partial x_j}) = SL^2\frac{\partial H}{\partial T} + \rho L^2\frac{\partial \eta}{\partial T}$$

Putting $t = \frac{T}{L^2}$, $\frac{\partial t}{\partial T} = \frac{1}{L^2}$ and

$$\frac{\partial H}{\partial T} = \frac{\partial H}{\partial t}\frac{\partial t}{\partial T} = \frac{\partial H}{\partial t}(\frac{1}{L^2})$$

$$\frac{\partial \eta}{\partial T} = \frac{\partial \eta}{\partial t}\frac{\partial t}{\partial T} = \frac{\partial \eta}{\partial t}(\frac{1}{L^2})$$

and finally, we have ,

$$\frac{\partial}{\partial x_i}(\hat{K}_{ij}\frac{\partial H}{\partial x_j}) = S\frac{\partial H}{\partial t} + \rho\frac{\partial \eta}{\partial t} \qquad (A)$$

2. Solute Transport Equation

$$\frac{\partial}{\partial X_i}(\hat{D}_{ij}\frac{\partial C}{\partial X_j}) - \frac{\partial}{\partial X_i}(V_j C) - C\frac{\partial \eta}{\partial T}\ \eta\frac{\partial C}{\partial T}$$

Where

$$\hat{D}_{ij} = \eta D_{ij}$$

$$V_j = \eta v_j$$

Non-dimensionalization

Defining new variables as $x_i = \frac{X_i}{L}, c = \frac{C}{C_0}$

$$\frac{1}{L^2}\frac{\partial}{\partial x_i}(\hat{D}_{ij}\frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i}(V_j c)\frac{1}{L} - c\frac{\partial \eta}{\partial T} = \eta\frac{\partial c}{\partial T}$$

Multiplying by L^2, it follows

$$\frac{\partial}{\partial x_i}(\hat{D}_{ij}\frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i}(V_j L c) - L^2 c\frac{\partial \eta}{\partial T} = L^2\eta\frac{\partial c}{\partial T}$$

Putting $t = \frac{T}{L^2}, \frac{\partial t}{\partial T} = \frac{1}{L^2}$ and

$$\frac{\partial c}{\partial T} = \frac{\partial c}{\partial t}\frac{\partial t}{\partial T} = \frac{\partial c}{\partial t}(\frac{1}{L^2})$$

$$\frac{\partial \eta}{\partial T} = \frac{\partial \eta}{\partial t}\frac{\partial t}{\partial T} = \frac{\partial \eta}{\partial t}(\frac{1}{L^2})$$

and finally, we have ,

$$\frac{\partial}{\partial x_i}(\hat{D}_{ij}\frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i}(V_j L c) - c\frac{\partial \eta}{\partial t} = \eta\frac{\partial c}{\partial t} \qquad \text{(B)}$$

Keeping H in its primitive form, the solution of equation (A) with H^1 continuity condition yields $\frac{\partial H}{\partial x_j}$ and using this gradient value directly in Darcy equation gives $V_j L\rho$. This value is computed as V_{xt} in the computer code which is to be used in the transport equation where we need $V_j L$ in the advection term.

For the evaluation of $D = \alpha' V^n$ with $n = 1$, we have

$$\hat{D} = \eta D = \eta V \alpha' = \frac{\alpha'}{L\rho} V_{xt}$$

To avoid L, we can define $\alpha = \frac{\alpha'}{L\rho}$ and for constant ρ, $\alpha = \frac{\alpha'}{L}$ which gives

$$\hat{D} = \alpha V_{xt}$$

APPENDIX - D

DESCRIPTION OF THE MODEL CONTROLLING PARAMETERS

CONTROLLING PARAMETERS FOR COMPUTER PROGRAMS

INDEX

= 0 Means Steady-State Condition,
Otherwise Unsteady

IGT

= 1 Means GWF-Equation,
= 2 TRANS. Equation,
= 0 Means Both Equations

IC

= 0 Not Coupled,
otherwise Coupled

IAGGR

= 0 Concentration-independent Parameters,
= 1 Concentration-dependent Parameters but without aggressiveness factor,
= 2 Concentration-dependent and Aggressive Case of Transport.

COMBINATIONS OF CONTROLLING PARAMETERS

TEST PROBLEM 01

INDEX =0
IGT=1
IC = 0
IAGGR = 0

Solves the GWF Equation in Steady-State Condition

TEST PROBLEM 02

INDEX =1
IGT=1
IC = 0
IAGGR = 0

Solves the GWF Equation in Unsteady-State Condition

TEST PROBLEM 03

INDEX =0
IGT=2
IC = 0
IAGGR = 0

Solves the Transport Equation in Steady-State Condition

TEST PROBLEM 04

INDEX =1
IGT=2
IC = 0
IAGGR = 0

Solves the Transport Equation in Unsteady-State Condition

TEST PROBLEM 05

INDEX =0
IGT=0
IC = 0
IAGGR = 0

Solves the Both Equation in Steady-State Condition seperately.

TEST PROBLEM 06

INDEX =1
IGT=0
IC = 0
IAGGR = 0

Solves the Both Equation in Unsteady-State Condition seperately

TEST PROBLEM 07

INDEX =0
IGT=0
IC = 1
IAGGR = 0

Solves the Both Equation in Steady-State Condition and coupled.

TEST PROBLEM 08

INDEX =1
IGT=0
IC = 1
IAGGR = 0

Solves the Both Equation in Unsteady-State Condition and coupled

TEST PROBLEM 09

INDEX =1
IGT=0
IC = 1
IAGGR = 1

Solves the Both Equation in Unsteady-State Condition and coupled and concentration-dependent parameters without aggressiveness factor.

TEST PROBLEM 10

INDEX =1
IGT=0
IC = 1
IAGGR = 2

Solves the Both Equation in Unsteady-State Condition and coupled and concentration-dependent parameters with aggressiveness factor.

TEST PROBLEM 11

INDEX =0
IGT=0
IC = 1
IAGGR = 1/2

Solves the Both Equation in State Condition and coupled and concentration-dependent parameters with / without aggressiveness factor.

APPENDIX - E

SAMPLE DATA INPUT

DESCRIPTION OF INPUT PARAMETERS FOR COMPUTER PROGRAMS

ALFA	Dispersivity
CB	Specified Boundary Values of Concentration
DC	Dispersion Coefficient
DELT	Time Step
FDC	Source Term in Transport Equation
FGW	Source Term in Groundwater Flow (GWF) Equation
H0	Initial Head Distribution
HB	Specified Boundary Values of Head
IAGGR	Model Controlling Parameter as Defined in Appendix-D
IBC1	Degree of Freedom prescribed at u/s boundary (for 1D)
IBC2	Degree of Freedom prescribed at d/s boundary (for 1D)
IBOUND(I)	ith Node on the Prescribed Boundary
IC	Model Controlling Parameter as Defined in Appendix-D
IDCT	Initial condition type for Transport equation
IDCTYP	0 for Constant Transport Parameters, Otherwise f(x)
IDIM	Problem Domain Dimension
IC	Model Controlling Parameter as Defined in Appendix-D
IGWT	Initial condition type for GWF equation
IGWTYP	0 for Constant GWF Parameters, Otherwise f(x)
INDEX	Model Controlling Parameter as Defined in Appendix-D
IPLOT	Plotting Data Generation Pointer
IPR	Print Control Pointer(0 for all calculations)
IPRC	Print Interval in time steps for transient problems
IRUN	Run Identification Number

ITMAX	Maximum Number of Iterations Allowed
M	Number of Collocation Points per element
MDOF(I)	Degrees of Freedom specified on IBOUND(I)
NBOUND	Number of Nodes on the Prescribed Boundary
NDOF	Number of Degrees of Freedom per Node
NN0	Ratio of Kinematic Viscosity
NPE	Number of Nodes per Element
NUMT	Maximum number of time steps to be simulated
NX	Number of Divisions in x-direction
NY	Number of Divisions in y-direction
PER0	Initial Hydraulic Conductivity
POR0	Initial Porosity
PP0	Fluid Density Ratio
REX	Value of Exponent 'r' in Equation (19)
RFAC	Relaxation Factor for Aggressive term
S	Storativity
THETA	Implicitness factor for Variables
THETM	Implicitness factor for Matrices
TITLE	Problem Description
TOL	Tolerance Limit for Convergence
VEL	Groundwater Velocity
XMAX	Maximum Value of x in the Domain
XMIN	Minimum Value of x in the Domain
XX	Collocation Point Factor
YMAX	Maximum Value of y in the Domain
YMIN	Minimum Value of y in the Domain

SAMPLE DATA INPUT FOR THE COMPUTER PROGRAM

Card	1	TITLE(20A4)
	2	IRUN, INDEX, IGT(3I5) TOL(E10.4) IDIM, IPR(2I5) S, ALFA(2E10.4), ITMAX, IAGGR(2I5)
	3	THETA, THETM, DELT(3E10.4), NUMT, NPE, IBC1, IBC2 IC, IPLOT(6I5)
	4	RFAC, REX(2E10.4)
	5	XX(E10.4)
	6	IGWTYP(I5)
	7	PORO, PERO, FGW, PP0(4E10.4)
	8	IGWT(I5)
	9	H0(E10.4)
	10 *to* 10+ NBOUND-1	IBOUND(I)(I5), HB(I)(E10.4), MDOF(I)(I5)
	10+ NBOUND	IDCT(I5)
	10+ NBOUND + 1 *to* 10 + 2*NBOUND +1	IBOUND(I)(I5), CB(I)(E10.4), MDOF(I)(I5)
	10 + 2*NBOUND + 2	IDCTYP(I5)
	10 + 2*NBOUND + 3	DC, VEL, FDC, NN0(4E10.4)

- All real variables are double precision

APPENDIX-F

EXPERIMENTAL STUDIES

INTRODUCTION

The behaviour of aquifer materials under different contamination levels is of vital importance for:

i) the study of flow dynamics of the system
ii) the prediction of contaminant movement in aquifers, and
iii) the management and proper disposal of contaminants

Among a number of aquifer parameters, the hydraulic conductivity is the fundamental one that defines the flow dynamics of the system since it is related to the velocity field and thereby, to the phenomena of hydrodynamic dispersion, the important process controlling the movements of contaminants in groundwater. Therefore, there exists a need to study the behaviour of aquifer materials under different situations. A complete study of the system includes:

i) the evaluation of aquifer parameters at different concentration levels of the contaminants
ii) the effect of aquifer material composition on different parameters
iii) effect of environmental factors on different parameters
iv) effects of change of flow conditions on aquifer parameters
v) effects of fluctuating source of contaminants (hystereses characteristics of the aquifer materials)
vi) behaviour of a water saturated aquifer when contaminants are introduced
vii) Behaviour of a contaminated aquifer due to change in contamination levels
vii) Kinetics of microorganism growth/decay and its affect on aquifer

parameters.

In a strict scientific sense, accurate and reliable modeling of flow and contaminant movement requires details of a complete study as outlined. Various types of investigations were reported in the related literature from different disciplines of science and technology. Most of those results are for general purpose oriented and they are not complete.

The compelling motive behind the proposed research was to study the flow dynamics of a contaminated aquifer by numerical experiments. The information required to express the hydraulic conducity as a function of concentration of the contaminants are available under certain conditions in the literature. The mathematical model proposed needs more information than available in literature. But it requires very sophisticated instrumentation as well as methodology. Unfortunately, such facilities are not available here at present.

Considering these constraints, such as the inherent problem of long time requirement, and the availability of resources, a simplified experimental scheme is proposed to study some of the possible features of the system.

The main objective of the experimental scheme was to study the flow dynamics of the system contaminated by aggressive solutes for saturated condition. The experimental model and the procedures are described in the following sections.

MODEL DESCRIPTION

The experimental model was made from transparent plexi glass tube with seven ports along its length. The experimental model is shown in figure-F1 . Different dimensions are listed in Table-F1.

TABLE-F1

Parameters	Dimensions
Length	40 cms.
Diameter(inside)	12.0 cms.
X-Sectional Area	114.98 sq.cms
Sample Length	30 cms.
Sample Volume	3449.4 cc.
Number of Ports	7
Distance between Ports	5 cms. c/c

MATERIALS AND METHODS

A set of combinations of sand, silt and clay contents will be evaluated to select two soil combinations giving suitable range of hydraulic conductivity to avoid the long time requirement.

Vertical circular columns (as described in Table-F1) with the provision of head measurements at uniform depth intervals will be used. In order to avoid compaction problem, an attempt will be taken to use the same circular columns as horizontal columns.

Head and concentrations will be recorded as a function of time and space whenever possible.

The three chemicals selected are NaCl , $FeCl_3$ and Phenol and a mixture of Natural Dune sand and Al-Qatif Clay was selected as packing material. There grain size distribution is shown in Figure-F2.

EXPERIMENTAL PROCEDURE

A. Preparation of Soil Sample

a) The homogeneous sand sample was obtained by taking the Dune sand particles passing through sieve number 10 and retaining on sieve number 20.

b) The sand content used in the sand-clay mixture was obtained from Dune sand passing through sieve number 10.

c) Required amount of silt-clay mixture (Al-Qatif Clay) passing through sieve number 100 was mixed with the dune sand (as described above). The sand-clay mixture is hand-mixed in dry condition to get a homogeneous sample.

B. Packing of the Columns

Because of the complexity due to the arrangements made for the study of the head diastribution pattern in the column, the vibration procedure was not used. Instead, hand compaction procedure was followed to obtain approximately uniform packing in the column. The hand compection procedure is summarized below:

a) The column length was devided into approximately ten layers. Material required for one layer was mixed with a suitable water content giving better workability. Wet packing also reduced the loss of finer particles as fine dusts during pouring into the column.

b) Each layer, one at a time, was filled with wet soil and compected with approximately 25 blows per layer with a round rubber hammar (Figure-F3).

C. Sample Saturation

The packed column was saturated with respective permeant starting slowly from the bottom layer.

Another advantage of saturation by reverse flow is to minimize the effects of entraped airs in voids inside the soil sample. The saturation process was continued for sometimes to allow the entraped air to be releazed. Saturation process was very slow since it was done for one layer at a time under a small head gradient to ensure small laminar flow. The sample saturation arrangement is illustrated in figure-F4.

D. Generation of Flow of Permeants

The most critical step of this experimental setup was to generate the flow through the packed medium inside the columns. Sudden opening as well as closing of the control valves might cause turbulence, sufficient enough to upset the system by the formation of channels (i.e. direct flow paths) inside the column. This channels were found to be prominent near the column walls.

The formation of excessive channels would creat direct flow paths , which will ultimately influence both the head distribution and the hydraulic conductivity of the system (figures from expt. no. 1).

In order to minimize this problem of turbulence, special H-Screw was fixed with the manometric tubes and the contoling valves were opened and closed gradually.

E. Flow Rate Adjustment

The flow rate Q is related to the hydraulic gradient and the relationship is presented by H. Darcy as

$$Q = -KA\frac{dh}{dl} \quad \text{-----(1)}$$

where Q = Volumetric Flow rate ($\frac{L^3}{T}$)

K = Hydraulic Conductivity ($\frac{L}{T}$)

A = cross-sectional area (L^2)

$\frac{dh}{dl}$ = hydraulic gradient ($\frac{L}{L}$)

The flow rate to be used in the present study was found to be of vital importance. Because the excessive flow rates from the outlet resulted with the development of suction affect in the ports. and ultimately the head distribution pattern was changed. This effect is discussed in the description of the first run. The proper adjustment of the flow-rate is very essential for the gravity flow. In this experimental study, the flow rate was adjusted by reducing the head gradient and/or by the adjustment of the outlet control valve.

METHODS OF PARAMETER DETERMINATION

1. Hydraulic Conductivity Measurement

The hydraulic conductivity of the medium was determined by using the wellknown Darcy's Law. Since uncertainty is the inherent problem with the measurement of any parameter- in porous media, a statistical approach is suggested by numerous investigators. Statistical averaging procedure was improved by minimizing the uncertainty involved in the system. This was accomplished by the additional advantage in the present study, e.g. the availability of the hydraulic gradient at different layers of the sample. This feature of the experimental model allowed to measure the hydraulic conductivity in between different ports and followed by suitable statistical approach to reflect, the degree of heterogeneity of the model.

In the calculation of the hydraulic conductivity, the following procedure was followed.

i) Several sets of head distribution data at different flow rates were selected

ii) The hydraulic conductivity K_d was calculated for each layer from the data in item (i) using the Darcy's Law, for each flow rate.

iii) The overall hydraulic conductivity K_0 was calculated using the total head drop in the system (i.e. between the two end ports) for each flow rate.

iv) A least squares fit was used to find the slope of the line between the hydraulic gradient and the flow rate, from which the representative hydraulic conductivity can be obtained. This procedure is illustrated in figur- e.

v) An alternative Straight-forward procedure can be applied which involves simple statistical averaging of the values obtained at different layers for each flow rate and followed by the application of least squares method.

2. Breakthrough Curve

The breakthrough curves were constructed for the calculation of the hydraulic conductivity at different concentration levels and to analize its nature at different clay contents and for different aggressive solutes.

When the effluent solute concentration approached the inlet concentration, the soil sample in the column was assumed to have constant concentration that is equal to the inlet concentration. The resulting hydraulic conductivity was taken as the hydraulic conductivity at the inlet concentration.

The effluent concentration was measured using curves of Figure-F5.

RESULTS AND DISCUSSIONS

The first test run was made with a homogeneous coarse sand sample. The hydraulic conductivity was measured by the procedure outlined earlier and the variation was practically negligible. The average hydraulic conductivity was found to be 24.35 cm/min and 15.03 cm/min for loose and compacted samples respectively. The flow rate-hydraulic gradient relationship is shown in figure-f6 which was in well agreement with the theoretical curve. The head distribution pattern was also in agreement with the theoretical one (Figure-F7).

When the mixture of sand, silt and clay was used as packing material, the saturation time was increased and permeability was decreased. This increased the observation time which resulted with uncontrolled microbial growth due to the presence of organic matters in the sample. As a result, flow siezed completely following one run (figure-8). In all other runs, the gradual growth of microorganisms and subsequent flow reduction were observed untill the pump failure occured. Analysis of the sample clearly demonstrated the microbial growth in the system, measured in terms of increase in volatile organic matters(figure-F9). Flow fluctuation was also observed with time and temperature indicating the predominancy of microbial growth in the system.

Although no change in sample size was observed, transient head distribution was noticed indirectly supporting the existance of the phenomenon of of incompressible unsteady flow condition due to the microbial growth and decay which change the medium porosity (Taylor et.al. 1990a,1990b, 1990c,1990d).

In the proposed mathematical model, microbial growth kinetics was not considered. Therefore, the correlation between the hydraulic conductivity and the solute concentration derived from a system where the microbial growth is predominant, is not feasible. Because, the magnitude of of the reduction of hydraulic conductivity by microbial growth is $5X10^{-4}$ as reported by Taylor et.al.(1990a,1990b, 1990c,1990d), where the the change due to concentration dependence is in the order of 180 as reported by Frankel et.al.(1977) and Abu Sharar (1987). It is obvious that the increase in hydraulic conducivity may be vanished at the begining of the microbial growth process. Since it was not possible to acheive at the steady state a breakthrough due to microbial growth interaction, it was not possible to further study the change in hydraulic conductivity with solute concentration , without considering the microbial growth kinetics. Since the increase in clay content increases the saturation time, bacterial growth is expected to be initiated during this time. A rapid saturation under high pressure upsets the soil sample inside the column.

The inherent problem of long time requirement and the predominent microbial phenomena made the experimental scheme unattainable. However, this study, was in agreement with the recent studies reported by Taylor et.al.(1990) and suggested by Khondaker et.al.(1990). It has paved the way to a potential area of future reaserch in which microbial growth kinetics could be included in the mathematical modeling of natural flow systems, particularly in modeling the fate and movement of organic compounds.

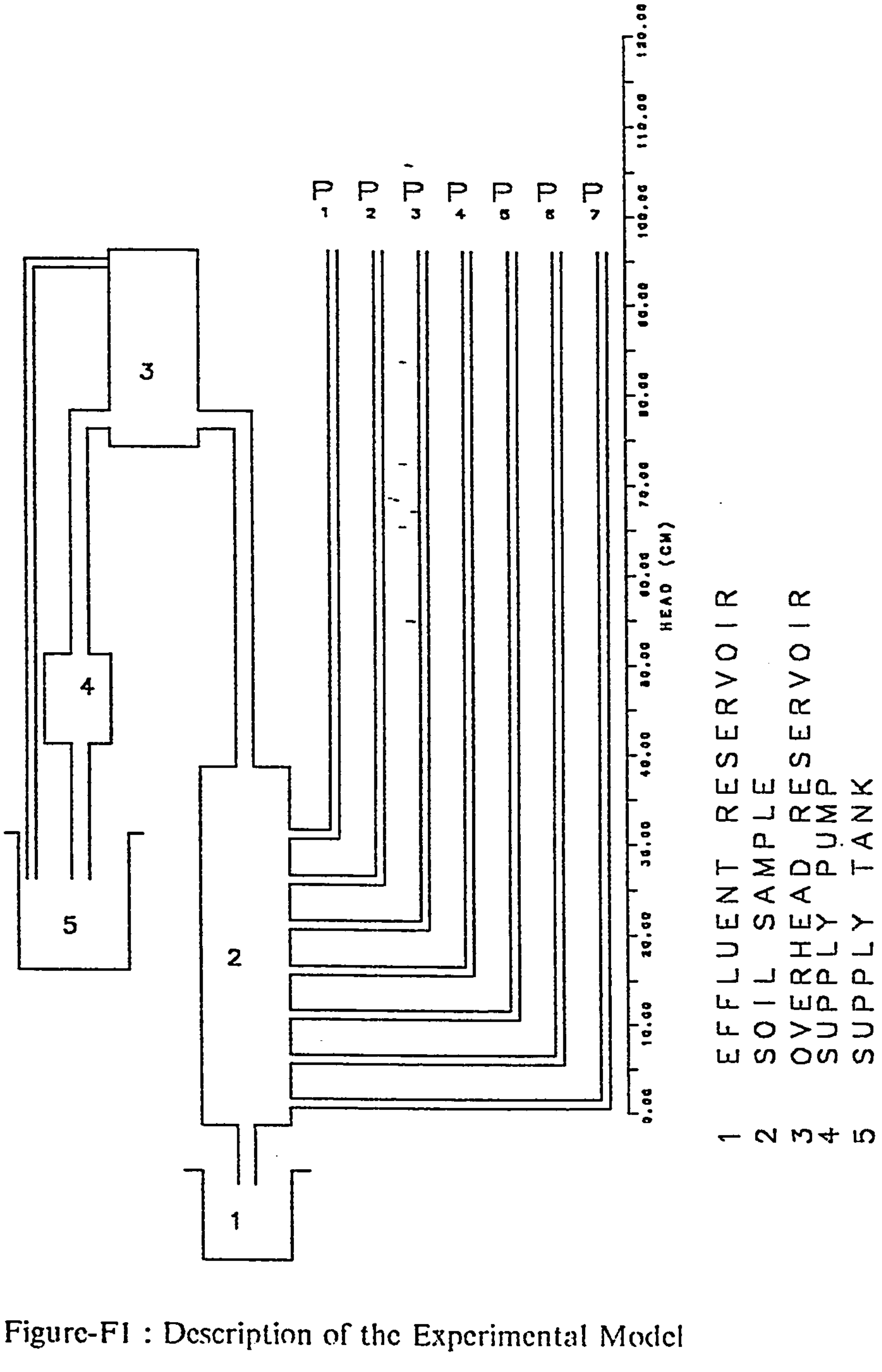


Figure-F1 : Description of the Experimental Model

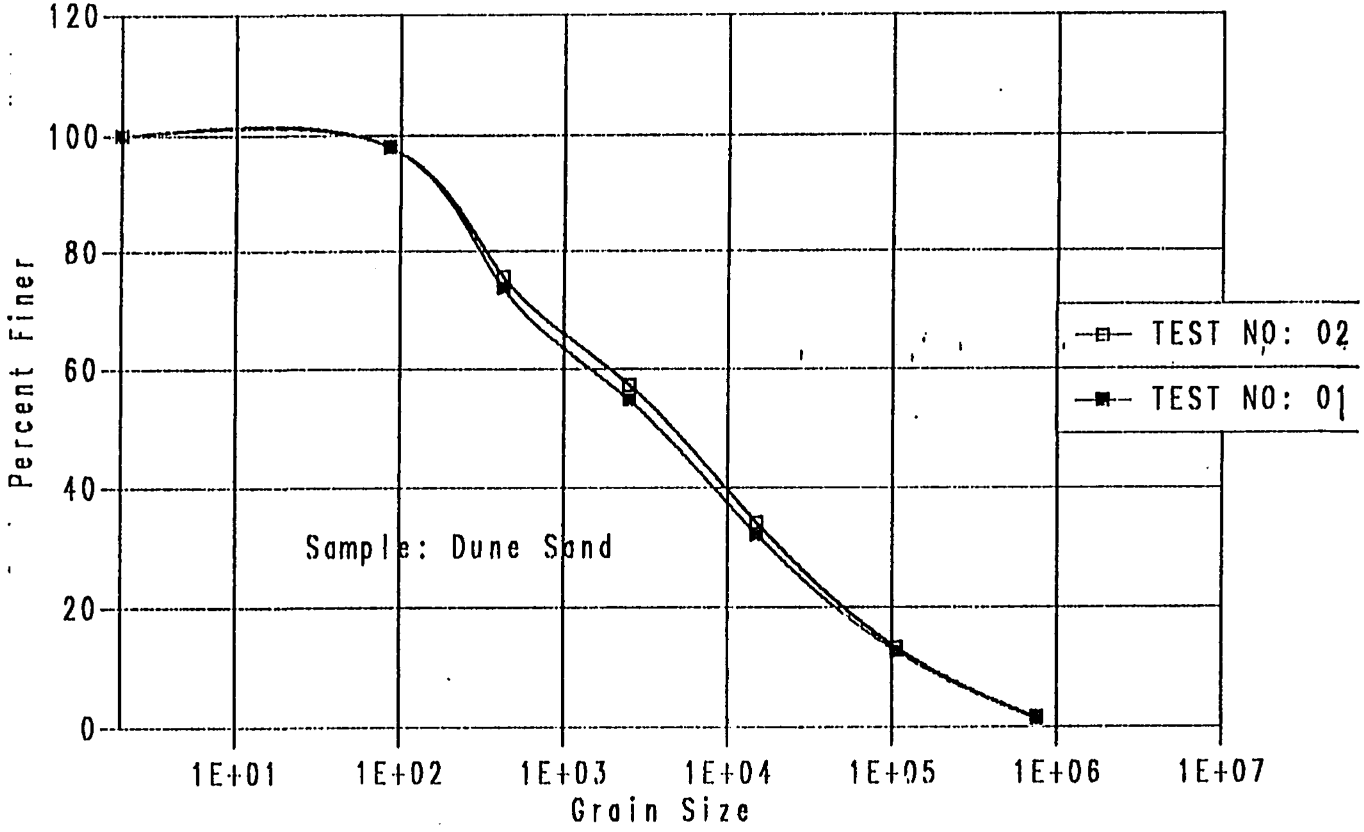


Figure-F2 : Grain size Distribution of Dune Sand

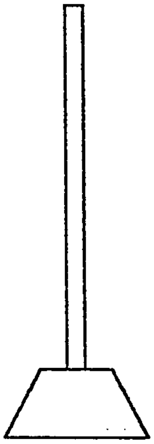


Figure-F3 : Circular Rubber Hammer used in hand Compaction

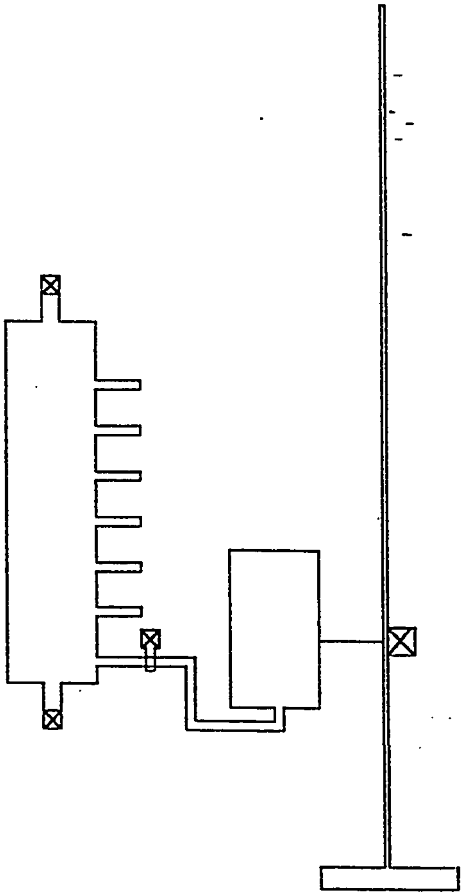
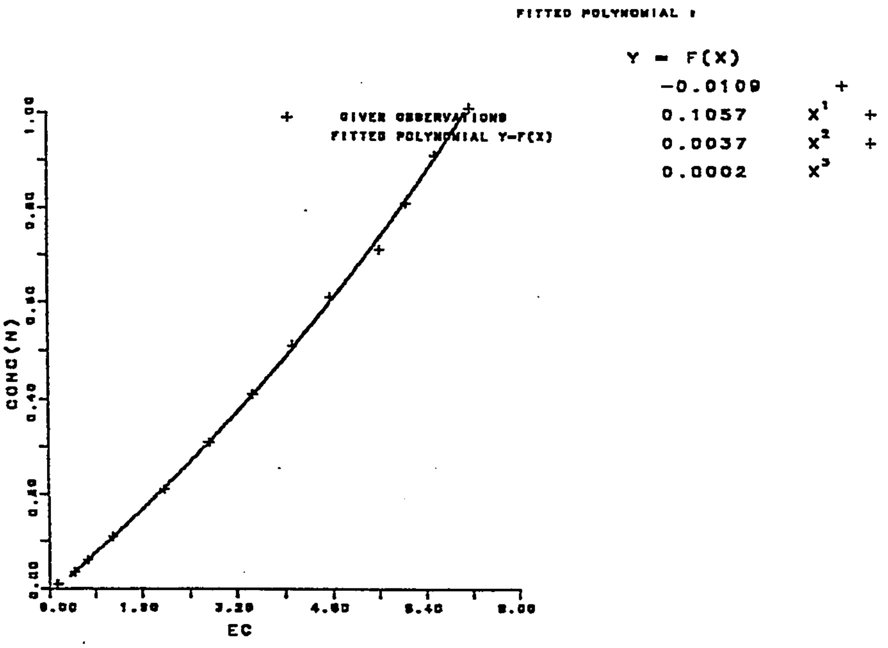


Figure-F4 : Sample Saturation Arrangement



```
FITTED POLYNOMIAL :

Y = F(X)
   -0.0109        +
    0.1057   X^1  +
    0.0037   X^2  +
    0.0002   X^3
```

Figurc-F5 : NaCl Concentration-EC rclationship

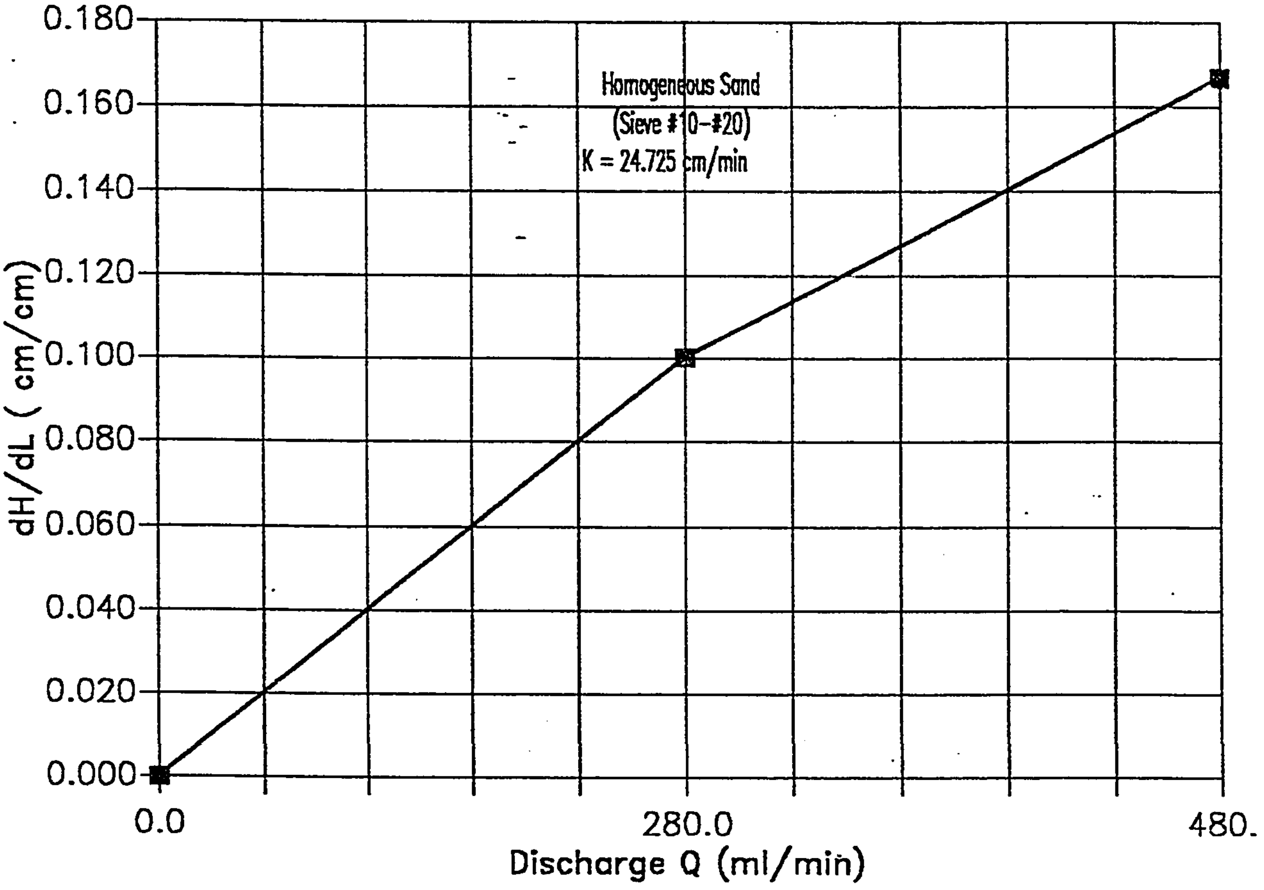


Figure-F6 : Discharge and Hydraulic Gradient relationship for homogeneous sand

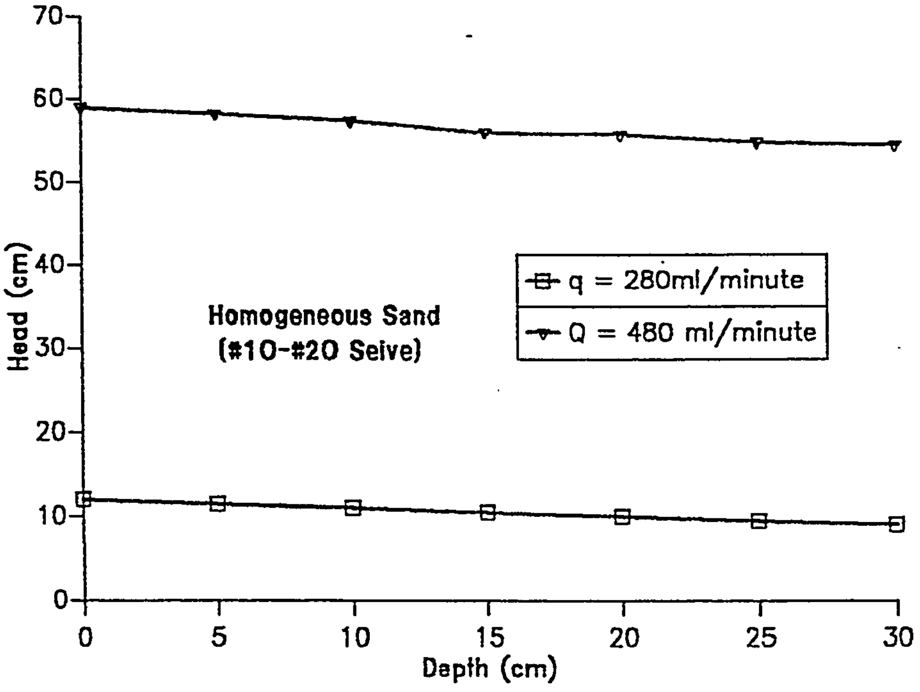


Figure-F7 : Head Distribution in homogeneous sand

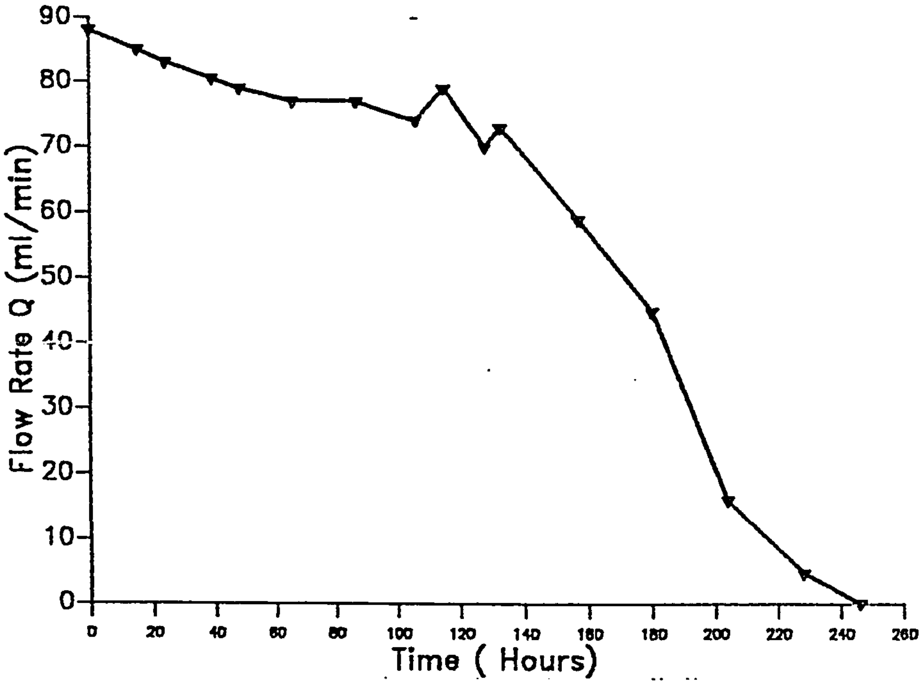


Figure-F8 : Flow Rate variation with time due to Microbial growth in Dune Sand sample

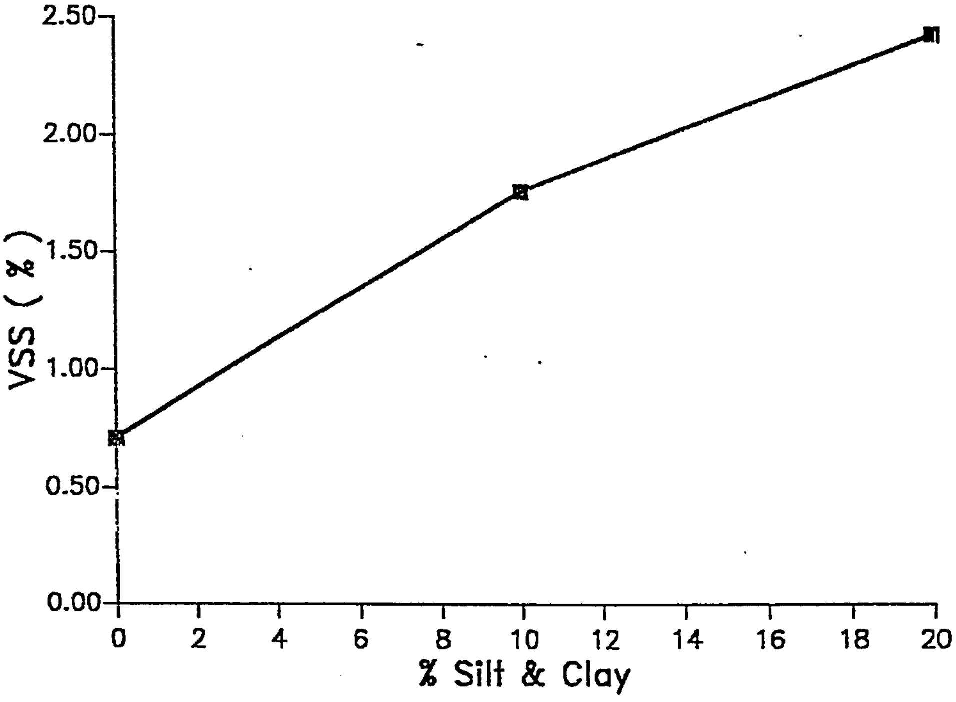


Figure-F9a : Volatile Organic Matter content and percent Clay relationship

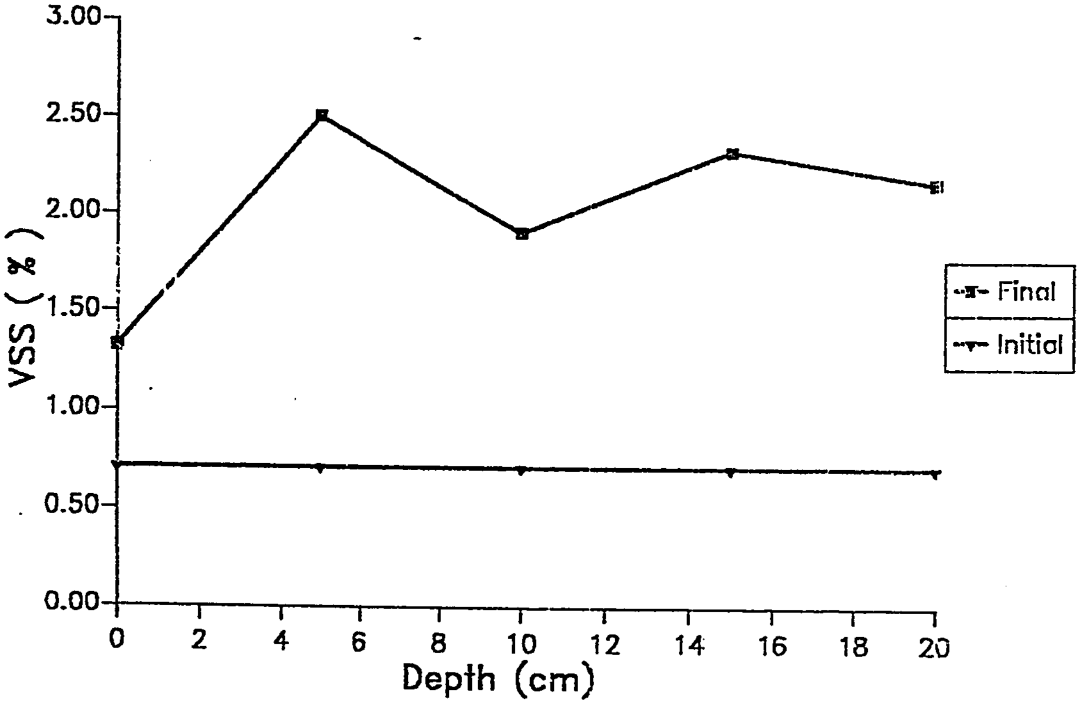


Figure-F9b : Bacterial growth in Dune Sand Sample

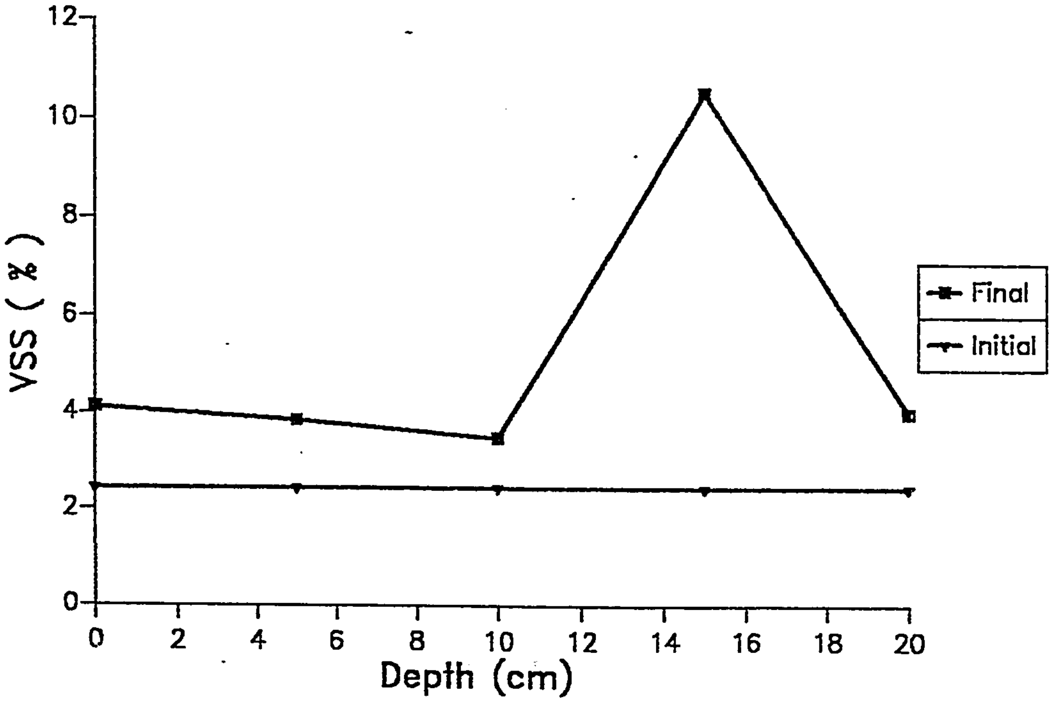


Figure-F9c : Bacterial growth in Dune Sand and 20 % Clay and Silt mixture

NOMENCLATURE

NOMENCLATURE

c	Solute Concentration $(\frac{M}{L^3})$
C	Dimensionless Concentration
D_0	Coefficient of molecular diffusion $(\frac{L^2}{T})$
D_x	Coefficient of hydrodynamic dispersion in x-direction $(\frac{L^2}{T})$
D_y	Coefficient of hydrodynamic dispersion in y-direction $(\frac{L^2}{T})$
g	Acceleration due to gravity $(\frac{L}{T^2})$
h	Hydraulic head (L)
K	Hydraulic conductivity $(\frac{L}{T})$
K_0	Hydraulic conductivity at concentration C_0 $(\frac{L}{T})$
p	Pressure (L)
t	time (T)
v	fluid velocity $(\frac{L}{T})$
x,y	Space variables in cartesian coordinate system (L)
α	Coefficient of Aquifer compressibility $(\frac{LT^2}{M})$
α_i	Dispersivity in ith direction (L)
β	Coefficient of compressibility of water $(\frac{LT^2}{M})$
η	Effective porosity
ξ	Local coordinate in x-direction
ζ	Local coordinate in y-direction
ν	Kinematic viscosity of the fluid $(\frac{L^2}{T})$

ν_0	Kinematic viscosity of the fluid at concentration C_0 ($\frac{L^2}{T}$)
ρ	Density of fluid ($\frac{M}{L^3}$)
ρ_0	Density of fluid at concentration C_0 ($\frac{M}{L^3}$)
ω	Solute mass fraction
γ	Empirical constant = 0.6923 for brine
μ	Fluid viscosity ($\frac{M}{LT}$)
μ_0	Fluid viscosity at concentration C_0 ($\frac{M}{LT}$)
κ	Intrinsic permeability (L^2)
κ_0	Intrinsic permeability at concentration C_0 (L^2)

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