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CONCEPTUAL MODELS FOR BIOLOGICAL CLOGGING OF UNSATURATED SOILS

By

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the Faculty of Graduate Studies and Research
in partial fulfillment of the requirements
for the degree of

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ABSTRACT

Clogging in the unsaturated zone is an important issue in the field of septic systems and biofilters. Different conceptual models for clogging in the saturated zone were proposed in the literature but corresponding conceptual models for clogging in the unsaturated zone are limited.

For this research, different conceptual models were proposed to relate the relative permeability of the soil with the microbial growth. The models vary from microscopic to macroscopic and from analytically derived to empirical. The models were formulated based on the approach proposed by Burdine (1953) and Mualem (1976) to estimate the value of the relative permeability as a function of the effective water saturation.

The proposed conceptual models were implemented in a one dimensional unsaturated flow and contaminant transport C++ code. The code uses Monod kinetics to simulate the microbial growth in the soil. Different verification data were used to verify that the equations were implemented correctly and a mass balance function for the flow and contaminant transport were implemented to check the code reliability. Also, different attempts were made to try to increase the confidence level in the proposed theoretical conceptual models.

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LIST OF SYMBOLS

A	cross section area (cm ²)
[A]	tri-diagonal matrix in Appendix A
a₁	summation of the advection and dispersion terms for grid block i-1
a₂	summation of the advection and dispersion terms for grid block i
a₃	summation of the advection and dispersion terms for grid block i+1
B	index in the input file for using Burdine's equation
b	cell decay coefficient (s ⁻¹)
C	concentration of the substrate (mg/L)
C	index in the input file for using central weighting
C_i^{t+Δt}	concentration at grid block i at time t+ Δ t (mg/L)
C_i^t	concentration at grid block i at time t (mg/L)
C_{i+1}^t	concentration at grid block i+1 at time t (mg/L)
C_{i-1}^t	concentration at grid block i-1 at time t (mg/L)
C₀	initial concentration (mg/L)
D[*]	effective diffusion coefficient (cm ² /s)
D_{i+1/2}	dispersion coefficient at the interface i+1/2 on Figure 3.12 (cm ² /s)
D_{i-1/2}	dispersion coefficient at the interface i-1/2 on Figure 3.12 (cm ² /s)
D_L	dispersion coefficient in the longitudinal direction (cm ² /s)
D_{AB}	diffusion coefficient (cm ² /s)
D_T	dispersion coefficient in the transverse direction (cm ² /s)
D_s	dispersion coefficient (cm ² /s)
dS/dP_c	gradient of the capillary pressure-saturation relationship

F	one-dimensional mass flux due to advection (mg.cm/L.s)
g	gravitational acceleration (cm/s ²)
H	index in the input file for using head as a boundary condition
h	total head (cm)
$h_w(z)$	total head for water at level z (cm)
$h_{w,i}$	total head for water at grid block i (cm)
$h_{w,i+1}$	total head for water at grid block $i+1$ (cm)
$h_{w,i-1}$	total head for water at grid block $i-1$ (cm)
$h_{w,1}$	prescribe total head boundary condition at the bottom of the column (cm)
$h_{w,n}$	prescribe total head boundary condition at the top of the column (cm)
i	grid block index
$K(\theta)$	unsaturated hydraulic conductivity or saturated hydraulic conductivity as a function of (θ) (cm/s)
K_s	half-velocity constant (mg _{substrate} /L)
K_{sat}	saturated hydraulic conductivity (cm/s)
$K(S_w)$	saturated hydraulic conductivity as a function of (θ) (cm/s)
$K(\theta)_{i+1/2}$	unsaturated hydraulic conductivity at the interface $i+1/2$ (cm/s)
$K(\theta)_{i-1/2}$	unsaturated hydraulic conductivity at the interface $i-1/2$ (cm/s)
$K(\theta)_{i\pm 1/2}$	unsaturated hydraulic conductivity at the interface $i \pm 1/2$ (cm/s)
k_r	relative permeability (cm/s)
$k_r(S_e)$	relative permeability as a function of the effective saturation
$k_r(S_{ew})$	relative permeability as a function of the effective water saturation
L	column length (cm)

M	index in the input file for using Mualem's equation
m	van Genuchten fitting parameter for capillary pressure-saturation relationship
M_T	microbial concentration (mg _{cells} /L)
N	index in the input file for using continuous loading
n	van Genuchten fitting parameter for capillary pressure-saturation relationship
n	last block on Figure 3.12
n_e	effective porosity
P	water pressure (cm)
P	index in the input file for using Pulse loading
P_b	bubbling pressure or the capillary fringe height (cm)
P_c	capillary pressure (cm)
P_{c1}	capillary pressure corresponding to a saturation of 0.125 on Figure 4.5 (cm)
P_{c2}	capillary pressure corresponding to a saturation of 0.375 on Figure 4.5 (cm)
P_{c3}	capillary pressure corresponding to a saturation of 0.625 on Figure 4.5 (cm)
P_{c4}	capillary pressure corresponding to a saturation of 0.875 on Figure 4.5 (cm)
Q	flow rate (cm ³ /s)
q	Darcy flux (cm/s)
q₁	prescribe flux boundary condition at the bottom of the column (cm/s)
q_m	maximum specific rate of substrate utilization (mg _{substrate} / mg _{cell} . s)
q_n	prescribe flux boundary condition at the top of the column (cm/s)

R	index in the input file for using Monod kinetics
R_s	source/sink term (mg/L . s)
r	radius of capillary tube (cm)
r_1	radius of capillary tubes covers 25% of the porosity on Figure 4.6 (cm)
r_2	radius of capillary tubes covers 25% of the porosity on Figure 4.6 (cm)
r_3	radius of capillary tubes covers 25% of the porosity on Figure 4.6 (cm)
r_4	radius of capillary tubes covers 25% of the porosity on Figure 4.6 (cm)
r_i	radius at number of divisions (i) (cm)
S_{am}	actual microbial saturation
S_{at}	actual total saturation
S_e	effective saturation
S_{em}	effective microbial saturation
S_{et}	effective total saturation
S_{aw}	actual water saturation
S_{ew}	effective water saturation
S_{trap}	effective entrapped air
S_w	water saturation
S_{wr}	irreducible water saturation
$S_{w,i}^{t+\Delta t}$	water saturation at grid block i at time $t + \Delta t$
$S_{w,i}^t$	water saturation at grid block i at time t
$T_{1/2}$	decay half life of a contaminant (s^{-1})
t	time (s)
th	biofilm thickness (cm)

U	index in the input file for using Upstream weighting
$U_o _0^{Porosity}$	constant represents the relative permeability term for Model #3 when there is no microbial activity involved
$U_i _0^{Porosity}$	constant represents the relative permeability term for Model #3 when there is microbial activity involved
V	seepage velocity (cm/s)
$V_{i+1/2}$	seepage velocity at the interface $i+1/2$ on Figure 3.12 (cm/s)
$V_{i-1/2}$	seepage velocity at the interface $i-1/2$ on Figure 3.12 (cm/s)
V_m	microbial volume
W	index in the input file for using flux as boundary conditions
$\{X\}$	vector in Appendix A
x	parameter used in Appendix A
Y	cell yield coefficient ($mg_{cell} / mg_{substrate}$)
y	parameter used in Appendix A
z	elevation head (cm)
α	van Genuchten fitting parameter for capillary pressure-saturation relationship (cm^{-1})
α_L	dispersivity in the longitudinal direction (cm)
α_T	dispersivity in the transverse direction (cm)
Δt	size of time step (s)
Δx	size of a grid block in the x direction (cm)
Δy	size of a grid block in the y direction (cm)
Δz	size of a grid block in the z direction (cm)
$\{\delta\}$	vector in Appendix A

$\partial h / \partial L$	hydraulic gradient along the flow path
ϕ	porosity
λ	Brooks and Corey fitting parameter for capillary pressure-saturation relationship
λ	first order decay rate coefficient in equations 3.36, 3.37, 3.38, 3.39 and 3.65 (s^{-1})
μ	dynamic viscosity (Pascal.s)
θ	volumetric moisture content
θ_r	irreducible moisture content
ρ	density (gm/cm^3)
$\rho_{dry\ bacteria}$	dry bacteria density (gm/cm^3)
ρ_w	water density (gm/cm^3)
σ	surface tension for water/air interface (dyne/cm)
τ	tortuosity
ψ	capillary pressure (cm)

1 INTRODUCTION

1.1 OVERVIEW

A large number of people in North America are living in areas not served with sewage facilities (Jawon 1976; Hagedorn et al. 1981). Septic tank systems are considered the most feasible way to treat wastewater in these areas (Kennedy 1998). Septic tanks and drainage fields are located in the soil zones that are close to the ground surface. This soil zone is the unsaturated zone and will be affected by the septic tank effluent. The soil in the unsaturated zone will be responsible for treating the septic tank effluent and it may clogs over time due to filtration and continuous microbial growth. Hence, clogging of unsaturated soils and how this clogging will affect the conductivity of the soil has to be understood in order to minimize the clogging problems and to use the soil in this zone as an effective treatment system.

Researchers have looked at clogging from three aspects: chemical, physical and biological mechanisms (Rice 1974). Chemical clogging is caused by the chemical reactions between the dissolved salts in the water which results in the formation of salt particles that precipitate between the soil particles and lower the permeability of the soil. Physical clogging is the result of suspended solids that physically block the pores and reduce the pore diameters which will lower the permeability. Biological clogging is due to growth of bacteria that attach to the solid particles and block the flow paths which lower the permeability (Rice 1974).

Biological clogging, which is the scope of this research, is the important clogging mechanism when we are dealing with septic tank effluent. Microorganisms or bacteria are already present in the soil and need a suitable environment to grow. This suitable environment can be summarized into two factors, physical and nutritional (biochemical) factors. Physical factors include moisture, hydrostatic pressure and osmotic pressure. Nutritional factors include availability of carbon, nitrogen, sulfur, phosphorus, trace elements such as copper, iron, zinc and cobalt and in some cases vitamins (Black 1999). Hence, the nutrient source will be from septic tank effluent, land application of municipal wastewater like biosolids or rain infiltrating through sanitary landfills.

Biological clogging is not a new concept. Allison (1947) started to look at the change in permeability with time due to microbial growth. Since 1949, when Monod developed his well known equation (Monod 1949), research has advanced more rapidly in this area to try to simulate the microbial growth.

Practically, the impact of biological clogging can be seen in various biofilter applications. Biofilters such as peat filters are one important application in this field. Peat filters are known to be a way to purify water that passes through them and they are relatively inexpensive as well (Kennedy 1998). They have already been used in field applications such as treating the septic tank effluent from a public school west of Ottawa, Ontario, Canada (Kennedy and van Geel 2001).

Although clogging of saturated soils has been studied by many researchers (e.g. Rice 1974; Okubo and Matsumoto 1979; Okubo and Matsumoto 1983; Oberdorfer and Peterson 1985; Mattison et al. 2002), limited research has been conducted to develop a conceptual model for unsaturated zone clogging. The relation between the microbial

growth and the relative permeability of the unsaturated zone is not well understood. Also, conceptual models for biological clogging in unsaturated soils have not been proposed or included in a numerical model to simulate clogging as proposed in this research. This research proposed three conceptual models illustrating how microbial growth may affect the relative permeability or the conductivity of unsaturated soils from theoretical, mathematical and numerical points of view.

1.2 RESEARCH OBJECTIVES

The scope of this research thesis concentrates on developing conceptual models to simulate biological clogging in the unsaturated zone and show how the microbial growth can affect the relative permeability of the soil and cause clogging. The conceptual models vary from microscopic scale to macroscopic scale and from analytically derived to empirical equations. The microscopic scale conceptual model was based on the assumption of a biofilm that covers the soil particles. The macroscopic scale models relate the growth of microbes with the relative permeability term and do not consider the distribution of the microbial growth at the microscopic scale.

These conceptual models were implemented in a one dimensional unsaturated C++ code to illustrate or emphasize that effect. The C++ code is divided into three main parts. The first part solves the flow equation with an iteration process using Newton Raphson and Thomas algorithms to solve the saturation and total head profiles of the soil. Then a one dimensional advection-dispersion equation is solved using a finite difference scheme to calculate the concentration profile of the substrate added. The code allows users to change between central and upstream weighting to overcome the sharp front

problem associated with contaminant movement. In the third part, a sink term or biodegradation term is added to the transport equation to simulate the biodegradation using first order decay or Monod kinetics. Operator splitting, which involves splitting the advection and dispersion terms from the biodegradation term, was chosen to solve the transport equation. Fourth order Runge Kutta integration was used to solve the biodegradation term when Monod kinetics is chosen to simulate the microbial growth.

Mass balance functions for the flow and transport equations are used to check whether the code is conserving mass or not. Also, different verification cases were used to check if the equations were implemented properly.

2 BACKGROUND

2.1 SATURATED/UNSATURATED ZONE SOIL

The saturated zone is defined by the soil layer below the water table. All the voids in this soil zone will be filled with water (Delleur 1999). Vadose zone is the soil zone above the water table where the soil voids might be filled with water, if they are close to the water table, or partially saturated. A capillary fringe exists directly above the water table where voids will be totally filled with water. The capillary fringe height depends on the soil type. Basically, granular soils with large particle sizes will tend to have a small capillary fringe in comparison to granular soils with smaller particle size. Above the capillary fringe, the soil is called the unsaturated zone where the voids are partially filled with water (Delleur 1999).

Clogging in both saturated and unsaturated soils are different because of the pore saturation. To model a clogging scenario, one should understand the difference between the flow and contaminant transport equations in the saturated versus the unsaturated zone. If we are dealing with the unsaturated zone, all the equations will be function of the soil saturation as the flow and transport will be governed by where the water is present within the soil.

2.1.1 FLOW EQUATION

In the mid 19th century, 1856, Henri Darcy introduced one of the most important relationships for flow in porous media, which is Darcy's law (Delleur 1999). Darcy's law is the only representative flow equation we know to represent the flow in the saturated

zone. In 1931, L. A. Richards carried this equation over to the unsaturated zone (Nielsen et al. 1972; Gardner 1971). Richards equation, which represents the flow in the unsaturated zone, is function of the saturation of the soil. Richards equation is known to be a highly nonlinear partial differential equation and several attempts were made to solve Richards equation as illustrated in the paper series by Philip starting in 1956 and Swartzendruber in 2000.

2.1.2 SOLUTE TRANSPORT EQUATION

It was reported that the theory of advection-dispersive transport could be attributed to the contributions of Bear (1961) studies (Zheng and Bennett 1995). Solute transport theory noticed a rapid development in the 1970s due to two main factors. The first was an increased interest in studying groundwater quality, which was reflected by the increased efforts for groundwater remediation to meet water quality standards. The second reason was the rapid development in the computer industry which allowed one to simulate the solute transport and predict the contaminant movement (Zheng and Bennett 1995).

The difference between the transport equation in the saturated zone and the unsaturated zone is that the water saturation term has to appear in the unsaturated solute transport equation. Also, it is already known that the transport equation can simulate the transport of a certain chemical or microbial movement if bacteria cells are involved.

In saturated soils, numerous studies were conducted on the transport of various chemicals (e.g. Nguyen et al. 1982; Angelakis and Rolston 1985). On the other hand, Ouyang and Zheng (1999) reported that little effort was done in terms of studying

dissolved chemical transport through unsaturated soils. Ouyang and Zheng (1999) developed a three-dimensional finite element model to try to address this issue and they concluded that there was not much data in the literature to verify their model results.

In terms of microbial transport, Schafer et al. (1998) conducted an experiment with a sand column equipped with facilities to measure the saturation and pressure of water in the column. The experiment was done to study the microbial transport under unsaturated conditions. They add an additional sink term for the fact that there is an air-water interface present. They conclude that transport of bacteria is reduced due to the bacteria tendency to attach to the air-water interface.

2.1.3 BACTERIAL OVERVIEW

2.1.3.1 BACTERIA GROWTH

Gaudy and Gaudy (1980) described in detail microbial growth and decay. They divide growth and decay into four main phases. Phase one is the lag phase of growth, where the new bacterial cells that are newly added to the environment start to adjust themselves to their new environment. During this period, bacteria cells might consume a significant amount of substrate but they have not begun the steady state replication yet. Phase one can be divided into two minor steps where during the initial stage, very little change will occur in the cell mass and during the second stage the growth rate will start to move toward achieving the exponential growth phase. Phase two is the exponential and declining phases of growth, where the bacteria cells will start to grow rapidly and then the growth rate declines. This phase ends when the rate of change in the microbial

population with time reaches zero. Phase three is the stationary phase of growth, where the essential nutrients start to disappear. During this phase, the majority of the bacterial cells remain alive. Once the nutrients deplete, bacteria cells start to turn into internal carbon sources and they may become substrates themselves to help the remaining cells stay in a living state. The time it takes this process to occur varies but in general, in heterogeneous populations the stationary phase is fairly short. The last phase, which is accelerating and decelerating phases of autodigestion, can be divided into two stages. The first stage is a relatively short phase during which the cells start to die at an accelerating rate. The second stage follows in which cells die at an exponential decelerating rate which takes a longer time to occur (Gaudy and Gaudy 1980).

2.1.3.2 MICROBIAL POPULATION AND CELLS NUMBERS

Wilson et al. (1983) conducted a study to evaluate the effect of depth on the indigenous microbial population and their ability to degrade a number of organic pollutants. They recovered samples from depths of 1.2, 3.0 and 5.0 meters at the margin of a small floodplain near Lula, Oklahoma and they found that these samples contained 3 to 9×10^6 cells per gram of dry material. Webster et al. (1985) measured 10^6 - 10^7 cells per gram of substrate material in subsurface samples from Oklahoma and Texas at depths of 2 to 9 m. Hence, it is common to assume that a significant microbial population exists in the upper soil horizon (0-10m). Also, cell concentration can be calculated by assuming that the wet weight of the cells is 10^{-13} gram/cell (Odencrantz et al. 1990) and knowing a particle density of the residence soil.

In terms of microbial cell density, a dry cell density can be calculated by assuming a 80% moisture content and an average wet bacteria cell density of 1.2 g/cm^3 (Baek et al. 1989; van Veen and Paul 1979). Robertson et al. (1998) suggest a dry density value for different bacteria types such as 1.39 g/cm^3 for *C. Oligotrophus* and 1.35 g/cm^3 for E-Coli.

2.1.3.3 DIFFERENT KINETICS FOR BACTERIAL GROWTH

Monod (1949 and 1958) was one of the early investigators to develop a fairly simple equation to represent biodegradation and microbial growth. The Monod equation relates the specific growth rate of a microbial population to the concentration of a limiting substrate (Bazin et al. 1976).

Researchers have used the Monod equation in the past decade in different ways. Atkinson and Davies (1974) started with the Monod equation and developed a pseudo-analytical equation that describes the diffusion problem with biochemical reactions in microbial films for a single limiting substrate. Different kinetics were developed by other researchers such as Moser and Teissier to simulate microbial growth (Powell 1967; Atkinson and Davies 1974).

2.1.3.4 CONCEPTUAL FRAMEWORKS FOR BACTERIAL GROWTH

Saturated soils can be represented by three phases. Mobile water, immobile water and solid phase (Fig. (2.1)). In cases where bacteria are present, an additional fourth phase is presented which is the biomass layer as shown in Fig. (2.1) (Baveye and

Valocchi 1989). Baveye and Valocchi (1989) present three conceptual frameworks that were developed by previous researchers to mathematically simulate the bacterial growth and the biological reaction of solutes in saturated porous media.

Figure 2.1- Schematic representation for saturated soil phases, taken from Baveye and Valocchi (1989)

The first conceptual framework was based on Monod's contribution in which bacterial growth was simulated from a macroscopic point of view. It was referred to as the strictly macroscopic model by Baveye and Valocchi (1989) or Monod's model by Odencrantz et al. (1990). No assumptions related to the bacteria distribution and configuration are made and the biodegradation kinetics are driven by the bulk concentration of the substrate added to the system (Baveye and Valocchi 1989; Odencrantz et al. 1990). Therefore, in simple terms, this conceptual way of thinking assumes a direct relation between the bacterial growth and the macroscopic soil properties (Fig. (2.2)).

The second conceptual framework, which was contributed by Molz et al. (1986), assumes that the bacteria cells grow in discrete colonies, termed microcolonies, of 10 to

100 organisms attached to the solid particles (Baveye and Valocchi 1989; Odencrantz et al. 1990).

Figure 2.2- First conceptual framework, taken from Baveye and Valocchi (1989)

These colonies were assumed to have a defined shape of cylinders with a defined radius and thickness. A diffusion boundary layer of certain thickness was assumed to separate the biomass from the bulk liquid (Molz et al. 1986; Baveye and Valocchi 1989; Odencrantz et al. 1990). By assuming a number of cylindrical colonies, Molz et al. (1986) assumed that the biomass growth in a porous medium occurred by allowing the number of colonies to increase or decrease depending on the substrate concentration or mass present and the electron acceptor utilized (Baveye and Valocchi 1989) (Fig. (2.3)).

The third conceptual framework, which was represented by Williamson and McCarty (1976a) and Rittmann and McCarty (1981) and named as the biofilm model, assumes that the bacteria cells are covering the solid surface uniformly with a film of uniform thickness. This film is assumed to have a certain density and constant surface area per unit volume (Baveye and Valocchi 1989; Odencrantz et al. 1990). Also, this film

isolates the solid from direct contact with the bulk liquid as the bulk liquid will be only in contact with the biomass which is in contact with the solid particles (Fig. (2.4)).

Figure 2.3- Second conceptual framework, taken from Baveye and Valocchi (1989)

Figure 2.4- Third conceptual framework, taken from Baveye and Valocchi (1989)

De Beer and Schramm (1999) mentioned that the biofilm behaviour required more knowledge and investigation in terms of microbial populations within the biofilm, as most of the studies used the “black box approach”. Researchers argued that the biofilm model is the more accurate representation than the macroscopic Monod-based model and the microcolony model. During the past decade, researchers used the biofilm model to simulate the bacteria growth in terms of its distribution.

Williamson and McCarty (1976*b*) used field data to verify their biofilm model to try to understand the factors that affect the biofilm growth rate and how this can be used in designing water treatment reactors. Rittmann and McCarty (1980*b*) used the fundamental model of biofilm to show its capability of predicting the performance of larger-scale film behaviour. Many other researchers such as McCarty et al. (1984), Suidan and Wang (1985), Bouwer and Cobb (1987), Suidan et al. (1987), Saez and Rittman (1988), Heath et al. (1990), Rittman (1990), Manem and Rittman (1990), Wirtel et al. (1992), etc. used this biofilm model to predict the biomass growth while seeking different goals.

Taylor and Jaffé (1990*a*) proposed new two models, the closed pore model and the open pore model. The closed pore model was similar to what was proposed by Williamson and McCarty (1976*a*) except the biofilm was assumed to conduct water and hence a pore could become filled (closed) with biomass but still conduct water. The open pore model was based on the biofilm concept however the biofilm thickness never exceeded a certain value due to the fluid shear stress that developed at the water-biofilm interface. Hence the pores never completely fill or clog. More details and explanation for both the closed and open pore models will be given in section 2.3 in this chapter.

2.1.3.5 SOLUTION TECHNIQUE ASSOCIATED WITH THE BIOLOGICAL SINK TERM

Microbial growth is dependent on the substrate concentration since the substrate acts as a food source for the microorganisms. The microbial growth rate can be simulated by any of the kinetics mentioned previously (i.e. Monod, Moser and Teissier). The substrate transport equation includes a sink term dependent on the microbial mass or concentration. Also, it is already known that the advection-dispersion equation is a partial differential equation and there are analytical solutions for this equation based on various assumed initial and boundary conditions. In addition, the equation can also be solved using numerical techniques such as finite difference and finite element (Zeng and Bennett 1995).

When a source or sink term such as biodegradation is added to the equation, additional techniques can be used to solve this complicated equation. The operator splitting technique is used to split the advection-dispersion equation into two parts and each one is solved separately. The first part will be the advection-dispersion part and it can be solved using the regular techniques mentioned before (i.e. finite difference or finite element) and the second part, which is the sink term that expresses the biodegradation, will be in a form of an ordinary differential equation that can be solved using techniques to solve ordinary differential equations such as the Runge Kutta method (Edwards and Penney 1994).

Wheeler et al. (1988) used the operator splitting technique in their BIOPLUS code to split the solute transport equation into three ordinary differential equations that can be

solved easily. The three equations were to solve for the hydrocarbon concentration, dissolved oxygen concentration and the microbial growth and decay.

The operator splitting technique proved its efficiency to deal with the advection-dispersion equation when the advection term dominates transport (Wheeler and Dawson 1988; Wheeler 1988; Li et al. 1992).

2.2 CURRENT RESEARCH INTEREST

During the past three decades, researchers have been conducting research in the area of biological clogging in saturated soils. There was a lack of research into the development of conceptual models for biological clogging in unsaturated soils. Baek et al. (1989) made significant progress in simulating the clogging of unsaturated soils with their numerical model, BIOSOIL. They simulated chemical and substrate movement in unsaturated soil and they concluded that the biomass that builds up in the soil system can be simulated as an increase of silt content. They proposed that silt can be seen as a very fine soil material that can simulate the microbial effect. They did not continue their research efforts in this area but they provided a starting point to explore this field. During the 1990's, there were no significant advancements in modelling the clogging process in unsaturated soil.

In 2002, Rockhold et al. published a review paper that highlighted some of the earlier studies on the change in the hydraulic properties due to microbial growth in saturated soils and they discussed the characteristics that should be taken into consideration when trying to model clogging phenomena in unsaturated soils.

2.3 BIOLOGICAL CLOGGING IN SATURATED SOILS

Many research studies have been conducted to develop conceptual models for biological clogging in saturated flow systems. Allison (1947) studied the effect of microorganisms on the reduction in the permeability under saturated conditions. A series of column experiment were conducted on three soils from different locations in California. Allison (1947) started with sterile columns to which distilled water was added to study the change in permeability. A reduction in the permeability was found at the beginning due to swelling or the transport of particles over time (Allison 1947; Frankenberger et al. 1979) then a noticeable increase occurred after the entrapped air was removed. Then a large reduction in the permeability occurred until the soil clogged. Allison (1947) concluded that the clogging occurred due to microbial clogging and not due to soil particle movement or any other physical causes.

McCalla (1950) conducted a series of column experiments to evaluate microbial effect on saturated silty clay loam at different temperatures. Twelve columns were used in this experiment and they were kept under saturated conditions by adding tap water daily with a sucrose concentration of 2%. Six columns were kept in a refrigerator at 45° F and the rest at the room temperature. McCalla (1950) noticed that the hydraulic conductivity of the columns that were kept at the room temperature was low. However, the other six columns kept in the refrigerator were high (McCalla 1950). McCalla (1950) also noted that there was an increase in microbial growth in response to an increase in sucrose loading when additional sucrose was added to the columns at room temperature. McCalla (1950) concluded that the room temperature was favourable for the microbes to grow versus the refrigerator temperature. Also, there was other evidence associated with

the microbial growth, which was gas generation. The results were confirmed with different types of soils and different types of organic sources. McCalla (1950) attributed the reduction in the soil conductivity caused by the bacteria to two reasons. The first reason was that microbes can produce gas or colloids that can restrict the water movement. The second reason was that microbial growth can disturb the soil structure due to decomposing or biodegrading the organic content.

Frankenberger et al. (1979) conducted laboratory experiments to study the effect of microbial growth on the hydraulic conductivity of a soil under saturated conditions and to look at the effect of nutrients and energy source on clogging. Frankenberger et al. (1979) reported the same trends in permeability as Allison (1947) in that there was an initial decrease in the permeability due to swelling or movement of particles followed by an increase due to removal of trapped air and a subsequent decrease in the permeability due to accumulation of microbial products. Also, they mentioned that the biological clogging was dependent on many factors such as the bacterial population, biological activity and nutrients, and energy sources supplied (Frankenberger et al. 1979).

Okubo and Matsumoto (1979) investigated the relation between the actual infiltration rate and the biological clogging under saturated conditions. They conducted an experiment on three saturated sand columns. The substrate used was added continuously during the experiment. Okubo and Matsumoto (1979) noticed that the dissolved oxygen level decreased rapidly at a depth of 2 cm from the top of the columns after the first 15 days of substrate dosing and became less than 1 mg/L. It increased again slightly after 26 days and became slightly more than 1 mg/L. At 5 cm depth, the dissolved oxygen concentration decreased rapidly as well but it increased rapidly later on

from 1.4 to 5.9 mg/L during the first 15 days and it reached a constant level after 26 days. They suggest that the aerobic microbial growth was the reason for this dissolved oxygen concentration reduction at the surface layer for the first 15 days. Also, they noticed a variation in the infiltration rate and they explained it in four stages. In the first stage, the infiltration rate decreased rapidly with the reduction in the dissolved oxygen which was due to aerobic microbial growth in the first 10 days. In the second stage, the infiltration rate was almost constant or increased slightly as the aerobic microbial growth was limited by the limited dissolved oxygen provided between the 10th day and the 20th day. The reduction in the dissolved oxygen caused the biodegradation to decrease and the microbial population to decrease as a result. In the third stage, the infiltration rate decreased rapidly again as the anaerobic microbial growth took place in the surface layer between the 20th day and the 30th day and during this period, the biological clogging developed under the anaerobic conditions. The last stage started from the 30th day and they noticed a slower decrease in the infiltration rate. They recommend at that point, if the case was a real groundwater recharge system, to remove the potential clogged surface layer before the infiltration rate starts to decrease in the last stage (Okubo and Matsumoto 1979).

Okubo and Matsumoto (1979) also developed an interesting model to simulate the biological clogging. The model development was based on Hagen Poisseuille's law. They simulated the voids as bundles of straight circular capillary tubes with the same diameter. The analysis of this model was based on two assumptions. First, the capillary tubes diameters will become narrow uniformly as the biological clogging develops and the

second assumption is that the reduction in the porosity is proportional to the accumulative discharge (Okubo and Matsumoto 1979).

An extension of Okubo and Matsumoto research was conducted in 1983 when they investigated the biological clogging during artificial groundwater recharge. They divided the biological clogging into three stages. The aerobic period, the transition period, which is a transition between aerobic and anaerobic, and the third phase is the anaerobic period.

Also, they divided the infiltration rate into three stages according to the changes in water quality, head losses and hydraulic conductivity of the soil. The infiltration rate decreased rapidly at the first 10 days due to microbial growth as indicated by the rapid reduction in the dissolved oxygen. Then the infiltration rate increased slightly in the following 10 days as the microbial growth became limited with the dissolved oxygen provided (transition period). After the 21st day the infiltration rate decreased rapidly again due to anaerobic conditions. These three stages led to the same conclusion they provided in 1979 that the clogging will occur in the top surface layer of the column under study.

Oberdorfer and Peterson (1985) reviewed the most significant causes of clogging from previous field studies conducted in aquifers. The major cause of clogging in the long term was due to the suspended solids associated with the injected substrate to the well. The second major cause of clogging is due to microbial growth at the face of the injection well and surrounding the injection area where microbes are in contact with the substrate injected. The presence of chemical processes had less impact on soil clogging. Also, clogging might occur due to entrapped air and bubbles from gas generated by the injection process.

Oberdorfer and Peterson (1985) considered those conclusions when conducting their experiment. They proved that these conclusions were less relevant for the study they proposed in the Hawaiian environment where they conducted their experiment. Oberdorfer and Peterson (1985) injected a secondary treated sewage effluent into a medium carbonate sand aquifer to study the causes of clogging. They found that the long term clogging was not due to suspended solids which contradicts with what they found in the literature. They found that the short term reduction in permeability in the first few days of injection was due to the suspended solids. At this point, the microbial cells had not started to grow yet and thus could not biodegrade the substrate added to the environment. After a few weeks, when microbes started to grow and establish colonies, two major changes had occurred. First, a noticeable decrease in the substrate suspended solids due to replication of microbes that removed much of the clogging that took place during the first few days. Second, the denitrifying bacteria became well established and produced nitrogen gas in the zone near the injection well and fewer amounts of those bacteria were found far from the injection location. Oberdorfer and Peterson (1985) repeated the injection to support their conceptual thought of that clogging scenario. However they mentioned that this is not the only possible scenario and further investigations should be conducted.

Taylor and Jaffé (1990a) conducted an experiment on a sand column to relate the permeability reduction with biological growth. They used methanol as a substrate and assumed the biofilm conceptual framework to simulate the biomass growth. They showed that a lower operating temperature than that used by Rittmann and McCarty (1980a) can be used to slow the kinetics of substrate utilization. Rittmann and McCarty (1980a)

showed that a temperature of 20° to 21°C was enough to achieve a steady state substrate removal. Taylor and Jaffé (1990a) used a temperature of 15°C to achieve the previous goal. Taylor and Jaffé (1990a) suggested that one of two physical models they proposed might be the cause of the permeability reduction. The first one was the closed pore model where they allowed the biomass to grow and fill the entire pore space of the medium. By this way, water will be assumed to flow through the biomass layer itself. Taylor and Jaffé (1990a) realized that if this is the case, the biofilm model that was first proposed by Williamson and McCarty (1976a) would not be applicable anymore. Taylor and Jaffé (1990a) suggested this model because it explained the measured constant permeability in the first 8 to 20 cm of their column.

The second physical model suggested by Taylor and Jaffé (1990a) was the open pore model where they assumed that the fluid shear stress will increase with the reduction in the medium permeability and the fluid shear stress will shear mass from the biofilm layer to keep the pore space open to conduct water. As the biofilm grows and the pore space decreases, the shear stress and velocity of the water will increase at the water-biofilm interface. When steady state is reached, a critical shear stress value will be reached as the rate of biomass removal due to shear will balance the net biofilm growth. At this point, the permeability will reach a constant level as they observed in the column experiment. Also, the biofilm will act as a second solid phase and this has to change the pore geometry and the dispersivity as well. Taylor and Jaffé (1990a) concluded that biological activities will tend to reduce the permeability of the porous medium by three orders of magnitude. They also concluded that the open pore model was a logical conceptual model to express the reduction in the permeability and that the physical

models are important to conceptualize the relationship between the biomass growth and reduction in permeability.

Taylor et al. (1990) proposed an analytical estimation of the permeability reduction caused by the biofilm growth in porous medium. Taylor et al. (1990) mentioned that although this was applied to saturated flow, a straightforward extension can be made for unsaturated flow. Three assumptions were made; the first assumption was that the soil was saturated with a single fluid. The second was to assume steady state flow and the final assumption was to neglect the biofilm permeability. In order to maintain saturated flow, an aerobic condition was assumed because under anaerobic conditions, biogas can be generated, accumulated and block the pores. Taylor et al. (1990) proposed a sphere model where they assumed that the porous media consisted of spheres of equal diameter. Based on this spherical model, they concluded that this clogging model was applicable only for homogenous and unconsolidated porous media. Also, they concluded that the permeability reduction was the greatest when the pore sizes were uniform.

Taylor and Jaffé (1990*b*) presented a model to solve the clogging problem in aquifers during the injection period of recharging the groundwater with an effluent or limiting substrate or nutrient. The model described the fate and transport of the substrate and biomass in the aquifer and it took into consideration the transport, growth and decay in both water and biofilm phases. While the problem was multidimensional, the general phenomena may be studied in a one dimensional form (Taylor and Jaffé 1990*b*). They calibrated the model using data provided by their experimental sand column (Taylor and

Jaffé 1990a). Taylor and Jaffé (1990b) suggested that with pulse loading, clogging process will be limited.

Also, in this study, Taylor and Jaffé (1990b) used the biofilm conceptual framework and they concluded that future research should be conducted in the filtration and adsorption of microbes by biofilm and to study the effect of the biofilm growth on the anisotropy of the soil.

2.4 BIOLOGICAL CLOGGING IN UNSATURATED SOILS

There was lack of research into the development of conceptual models for biological clogging in unsaturated soils. Mainly, research has focused on field or laboratory work to study the effect of septic tank effluent on filters (e.g. sand filters).

Clement et al. (1996) proposed a macroscale model that does not assume any specific pattern for the microbial growth and just estimates the average biomass concentrations. Clement et al. (1996) mentioned that in reality, bacteria will grow first in discrete colonies then gradually expand to form a continuous biofilm layer covering the solid particles (Clement et al. 1996; Rittman 1993). Hence, the more general macroscale approach of how bacteria will grow is more realistic than the biofilm model as it assumes average biomass concentrations. Also, Darcy's law and the soil properties used in modelling transport process were based on a continuum scale which matched the macroscale assumptions. Clement et al. (1996) also mentioned that it was a costly process to measure the biofilm thickness of the microcolonies in reality and these processes are always associated with experimental errors.

Kristiansen (1981*a*) conducted an experiment using three trench sand filters (A, B and C) to illustrate the relationship between clogging and the physical and chemical environment of sand filters. The investigation was conducted for 17 months from July 1976 until November 1977. Trenches A and C were loaded with septic tank effluent at a rate of 4 to 6 cm/day and trench B at a rate of 12 to 18 cm/day. The temperature was between 4° and 16°C for trenches B and C and between 12° and 15°C for trench A. Kristiansen (1981*a*) found that the septic tank effluent accumulated in the sand filters as they started to clog and ponding started to occur. Pond rates, expressed as the filter area covered by ponding overtime, of 0.33, 0.27 and 0.16 m²/month were found in trenches A, B and C respectively. After 8 months from the beginning of the loading, the septic tank effluent ponds covered about 80, 67 and 40% of the filter surface area in trenches A, B and C respectively. After 15 months, the entire top surface area of the filter was covered by ponding effluent in trenches A and B but only 75% of the top surface area was covered in trench C. Kristiansen (1981*a*) suggested that the temperature might have different effects in different phases of clogging. Raising the temperature may have little effect on the accumulation of suspended soils in the voids but it has major effect in forming cement of particles that may clog the smaller soil pores (Kristiansen 1981*a*).

Kristiansen (1981*b*) continued his study on the fate of nitrogen and he found that an insignificant amount of nitrogen had been removed from the septic tank effluent passing through the sand filters but the nitrification process was significantly affected in the cold season.

Also, Kristiansen (1981c) studied the microbial growth and concluded that the number of microbial cells increased from an initial amount of 10^6 to $10^7 - 10^8$ per gram of dry sand due to loading with septic tank effluent.

Seki et al. (1998) conducted an experiment on three columns to verify the effect of bacteria and fungi on clogging, and reducing the hydraulic conductivity and infiltration rate of the soil in experimental columns. Three 5 cm diameter by 1 cm height columns were filled with a soil consisting of 15% clay, 35% silt and 50% sand. The column height was chosen to be very small because previous studies mentioned that biological clogging occurred within the first centimeter from the inlet of the injected substrate or nutrient (Rice 1974). Glucose solution was used as the substrate in one of the columns. The other two columns were dosed with glucose and different solutions to kill the bacteria in the second column and kill the fungi in the third column.

Seki et al. (1998) concluded that when fungi were killed, bacteria clogged the pores and vice versa. Microbial clogging was faster than fungal clogging which suggested that the fungi grew more slowly than bacteria. The volume of biogas produced by the bacteria reached its maximum value after 103 days from the time they added the glucose. The amount of gas produced blocked the water path which results in a reduction in the hydraulic conductivity. They concluded that the main two reasons for the hydraulic conductivity reduction were biological clogging and gas generation.

Or (2002) provided an overview of microbial activities in unsaturated soils at the microscale. He looked at the physical processes and criteria affecting the environment of the microbial community. Also, he studied the effect of the microbial activities on the soil structure, ability of the soil to transport fluids and soil pore space.

Or (2002) showed that at the microscale, the position and structure of the microbial colonies within the pore diameters will affect the diffusion and adsorption processes. Or (2002) claimed from literature that in microscopic observations of biological clogging systems, studies indicated that a continuous biofilm will be formed and cover the solid phase continuously or discrete microcolonies will be developed and clog the pore diameters randomly. Also, some observations that were made in a two dimensional glass network used for a microscale model study showed that biomass will form both a biofilm covering the solid phase and discrete microcolonies that will be randomly distributed and clog the pore throats as well (Or 2002). Also, Or (2002) reported that the transformation to a state of indigenous decay will result in partial biofilm movement and recovery in the hydraulic conductivity.

Spychata and Blazejewski (2003) conducted an experiment on a series of sand columns to study the conditions and factors that affect the clogging in fine sand with septic tank effluent based on physical modelling. Twelve columns were dosed with 82 mm/day preliminary treated septic tank effluent. The outflows from the twelve columns were connected to a main outflow exit. A reduction in the total discharge rate from the twelve columns was observed over the experiment period (from August 2000 until March 2002) at the same running temperature of 20°C. Only six columns remained unclogged until the end of the experiment (March 2002) but the rest were clogged after 480 days in December 2001.

Spychata and Blazejewski (2003) found from the vertical distribution of the organic matter that over 40% of all organic mass was found in the top 2.5 cm of the sand columns. The main reason for clogging was the high concentration of the microbial

population in this upper soil layer. The clogging process was accelerated with more suspended solids which were larger in size versus the soil pores. These suspended solids tremendously reduce the number of sand pores contributing to flow in the top layer of the sand filters.

Rockhold et al. (2002) reviewed some of earlier research conducted on microbial growth that changes the hydraulic properties of porous media. They found that most of the research was focused on saturated porous media and that this issue was not fully addressed in unsaturated soil systems. Rockhold et al. (2002) discussed the characteristics of unsaturated soil systems that might be important when modelling the microbial growth. Rockhold et al. (2002) concluded that microbial growth results in the reduction of the permeability and the porosity of soils. They claimed that the characteristics of biomass accumulated depended on the organic substrate added to the system, the loading rate of this substrate, the type of bacteria and the flow rate of the fluid.

Rockhold et al. (2002) mentioned that unsaturated soil systems are much more complex than saturated systems as the hydraulic conductivity and the water content are nonlinear functions of the capillary pressure. More difficulties are associated with the presence of the air/water interface in unsaturated systems in comparison with saturated systems.

As bacteria metabolize the substrates added to the system, gas is generated and becomes entrapped. This process noticeably reduces the hydraulic conductivity in both saturated and unsaturated soil systems (Rockhold et al. 2002).

2.5 SUMMARY

A large amount of research has been conducted to develop conceptual models for biological clogging in saturated soils. However, in comparison, a limited amount of research has been conducted to develop conceptual models for clogging in unsaturated soils.

Bacteria type, the organic substrate consumed, temperature, the pore space distribution, gas generation and other parameters affect the clogging in a porous medium. The macroscale models are the more representative of reality as they look at the problem from a continuum approach as the flow and transport equations and soil properties do. There is still a need to explore clogging of unsaturated soils to develop a well defined relationship between microbial growth and the macroscopic properties of the soil.

3 THEORETICAL AND CONCEPTUAL DEVELOPMENTS OVERVIEW

3.1 UNSATURATED ZONE THEORY DEVELOPMENT

3.1.1 INTRODUCTION

The unsaturated zone is the soil zone between the top of the capillary fringe and the ground surface. Above the capillary fringe or tension saturated zone, not all the pores are filled with water versus the capillary fringe and saturated zone below the water table where all the pores are filled with water (Fig. (3.1)).

The solid particles in the unsaturated zone are surrounded by thin film of water held by the adhesion and cohesion forces (James et al. 1999). Near the water table, water is held by capillary forces. Depending on the soil type, the capillary fingering might extent from few millimeters for large diameter soil particles to hundreds of centimeters for fine soil particles.

Figure 3.1- Definition of unsaturated and saturated zones

Since the unsaturated zone is above the water table, the water pressure is negative for static conditions with respect to atmospheric pressure. In this zone, we can represent the pores as series of capillary tubes with different diameters representing the different pore sizes. The capillary pressure varies inversely with the radius of the tube as,

$$P_c = \psi = \frac{2\sigma}{r} \quad (3.1)$$

where P_c or ψ is the capillary pressure, σ is the surface tension and r is the radius of the capillary tube.

Total head (h) at any point in the unsaturated zone will be the summation of the elevation head at that point (z) and the water pressure; knowing that the water pressure above the water table is negative, therefore;

$$h = z + \frac{P}{\rho g} \quad (3.2)$$

$$\text{since } P_c = -\frac{P}{\rho g} \quad (3.3)$$

$$h = z - P_c \quad (3.4)$$

where ρ is the density of the liquid, P is the water pressure, P_c is the capillary pressure, expressed as a height of water column, assuming the air phase pressure is zero, and g is the gravitational acceleration. Fig. (3.2) shows the relation between capillary pressure and saturation in the unsaturated zone. The reader should note that there are many relationships in the literature that describe this nonlinear relationship between capillary pressure and saturation in the unsaturated zone.

Figure 3.2- Capillary pressure versus saturation

3.1.2 BROOKS AND COREY VS. VAN GENUCHTEN

Two well known relationships by Brooks and Corey (1964) and by van Genuchten (1980) are commonly used in studying flow in the unsaturated zone.

Brooks and Corey (1964) relate saturation with capillary pressure and bubbling pressure or the capillary fringe height as follows:

$$S_{ew} = \frac{S_{aw} - S_{wr}}{1.0 - S_{wr}} = \left(\frac{P_c}{P_b} \right)^{-\lambda} \quad (3.5)$$

where S_{ew} is the effective water saturation, S_{aw} is the actual water saturation, S_{wr} is the irreducible water saturation, P_b is the bubbling pressure and λ is the pore size distribution index. P_b , as defined by Brooks and Corey (1964), is a measure of the maximum pore size forming a continuous network of flow channels and λ is a fitting number that characterizes the pore size distribution. λ is a positive number greater than zero. Depending on the media, λ is relatively small for media having a wide range of

pore sizes (e.g. well graded sand) and large for uniform pore size media (e.g. well sorted sand) (Brooks and Corey, 1964) (Fig. (3.3)).

Figure 3.3- Brooks and Corey capillary pressure – saturation relationship

In the van Genuchten (1980) relationship, different parameters have been used representing the different soil types and the surface tension at the solid particles.

The van Genuchten (1980) relationship is as follows:

$$S_{ew} = \frac{S_{aw} - S_{wr}}{1.0 - S_{wr}} = \left[1 + (\alpha P_c)^n \right]^{-m} \quad (3.6)$$

and

$$m = 1 - \frac{1}{n} \quad (3.7)$$

where α , n and m are fitting parameters. Often Eq. (3.7) is used to relate n and m . The parameter n reflects the curvature of the capillary pressure-saturation relationship and α reflects the height of the curve (Fig. (3.4)).

Figure 3.4- Effect of van Genuchten parameters on the capillary pressure saturation relationship

3.1.3 ACTUAL SATURATION VS. EFFECTIVE SATURATION

There are two ways of expressing the relation between the capillary pressure and the saturation. First, using the effective saturations (i.e. as shown in Fig. (3.4) if van Genuchten relationship is used) or using the actual saturations (Fig. (3.5)).

The difference between those representations is the irreducible saturation. In the effective saturation, the capillary pressure saturation relationship is scaled from zero to one. The irreducible saturation represents the thin layer of water that covers the solid particles and cannot be extracted except if a very high capillary suction is applied on the soil. Numerically, at that saturation, the gradient (dS/dP_c) approaches zero (Fig. (3.5)).

Figure 3.5- Irreducible saturation

3.1.4 PORE DISTRIBUTION, FLOW IN UNSATURATED ZONE AND RELATIVE PERMEABILITY

The shape of the capillary pressure-saturation curve is a function of the pore size distribution of the soil. If the soil is viewed as a bundle of capillary tubes of varying diameters, the capillary rise in each tube is a function of its radius as indicated in Eq. (3.1). If all the tubes were of similar diameter (e.g. well sorted sand), then the capillary pressure-saturation curve would be flat and the saturation would sharply decrease as the capillary pressure exceeds the capillary rise. If the bundle of tubes are at varying diameters (e.g. well graded sand), the change in saturation with a change in capillary pressure will be gradual. Fig. (3.6) can be used to illustrate this concept. If a soil is saturated, all the pores are filled with water. If suction is applied, the largest pores drain first because they have the lowest capillary pressure. As the suction continues to increase,

smaller and smaller pores start to drain. At very high suction or capillary pressure, only the smallest pores are filled.

Figure 3.6- Pores distribution with depth according to van Genuchten relationship

The flow equation in the saturated zone can be written as follows:

$$q = \frac{Q}{A} = -K_{sat} \cdot \frac{\partial h}{\partial L} \quad (3.8)$$

where q is the specific discharge or the volumetric flow rate per unit area of the porous medium perpendicular to the direction of the flow, Q is the flow rate, A is the cross section area, K_{sat} is the saturated hydraulic conductivity and $\partial h / \partial L$ is the hydraulic gradient along the flow path (Delleur 1999). It should be noticed that q is the *Darcian velocity* or the *Darcy flux* which is not the actual *average linear velocity* or the *seepage velocity* of the flow through the porous medium. The seepage velocity can be given as,

$$V = \frac{q}{n_e} \quad (3.9)$$

where V is the seepage velocity and n_e is the effective porosity. The effective porosity represents the pores that actually contribute to flow. In some soils, such as peat, which has a highly porous structure, a large number of dead zones exist which do not contribute to flow. Two porosities will be considered for those kinds of soils, the total porosity which represents the entire pore space and the effective porosity which represents only the pores that contribute to flow (Kennedy 1998; Delleur 1999).

The same flow equation (i.e. Eq.(3.8)) can be applied in the unsaturated zone taking into account saturation. The flow equation in the unsaturated zone is as follows,

$$q = -K(\theta) \cdot \frac{\partial h}{\partial L} \quad (3.10)$$

where $K(\theta)$ is the hydraulic conductivity as a function of θ and θ is the volumetric moisture content. This term can be written as,

$$K(\theta) = K_{sat} \cdot k_r \quad (3.11)$$

where k_r is the relative permeability. The relative permeability term is one of the most important terms when evaluating flow in unsaturated soils and the core of this research. It represents the conductivity of the pores that are contributing to the flow at certain saturation. Relative permeability varies from zero to one as illustrated in Fig. (3.7).

Figure 3.7- Relative permeability versus effective water saturation

3.1.5 RELATIVE PERMEABILITY

Burdine (1953) and Mualem (1976) equations are well known relationships that are widely used in the literature to relate the saturation with the relative permeability.

In 1953, Burdine developed an integral equation that expresses the relation between the relative permeability and saturation of the soil,

$$k_r(S_e) = S_e^2 \frac{\int_0^{S_e} \frac{dS_e}{\psi^2}}{\int_{S_e=0}^1 \frac{dS_e}{\psi^2}} \quad (3.12)$$

where $k_r(S_e)$ is the relative permeability, S_e is the effective saturation and ψ is the capillary pressure.

In 1976, Mualem derived another integral formula, that gives a relation between the relative permeability and saturation of the soil,

$$k_r(S_e) = S_e^{\frac{1}{2}} \left(\frac{\int_0^{S_e} \frac{dS_e}{\psi}}{\int_{S_e=0}^1 \frac{dS_e}{\psi}} \right)^2 \quad (3.13)$$

Both relationships integrate the expression over the saturated portion of the capillary pressure saturation curve $\left(\int_0^{S_e} \frac{dS_e}{\psi} \right)$ over the entire curve $\left(\int_{S_e=0}^1 \frac{dS_e}{\psi} \right)$ (Fig. (3.8)).

The van Genuchten relationship can be used to represent the capillary pressure-saturation relationship with the following expressions for the relative permeability terms.

For Burdine
$$k_r(S_{ew}) = S_{ew}^2 \left(1 - (1 - S_{ew}^{1/m})^m \right) \quad (3.14)$$

For Mualem
$$k_r(S_{ew}) = S_{ew}^{1/2} \left(1 - (1 - S_{ew}^{1/m})^m \right)^2 \quad (3.15)$$

The full integrations are provided in Appendix A.

Figure 3.8- Capillary pressure – saturation relationship “Water Saturation” based on Burdine (1953) and Mualem (1976).

For the biological clogging models proposed herein, the impact of the microbial growth on the permeability of the soil is incorporated into the relative permeability-saturation relationship. Those proposed conceptual models for clogging will be discussed in detail in the next chapter.

3.2 CODE DESCRIPTION AND NUMERICAL SOLUTION

3.2.1 INTRODUCTION

The proposed code solves the one dimensional, unsaturated flow and contaminant transport equations for the vertical direction. Different sink terms were added to the contaminant transport equation to simulate biodegradation. Simple first order kinetics was included to simulate the first order decay of a contaminant with time. Monod kinetics was included to simulate biodegradation coupled with microbial growth and decay. Further explanation of the biodegradation models is provided in the following subsections. A mass balance was incorporated into the model for the flow and contaminant transport equations to ensure that the solution conserves mass. The finite difference approximation was chosen as the numerical technique to solve both the flow and contaminant transport equations. The code assumed a constant grid size, constant temperature and constant fluid density. The coordinate system used was positive upwards with an assumed datum at the base of the model domain.

3.2.2 FLOW EQUATION AND METHOD OF SOLUTION

3.2.2.1 FLOW EQUATION

There are two ways to express the flow equation in the unsaturated zone, one using the control volume approach and the other using Richards equation (Philip 1956; Gardner 1971).

The unsaturated flow equation developed using the control volume approach has two unknowns, pressure head and saturation. To solve this equation, the code has to be supplied with a relation between pressure head and saturation to solve two equations with two unknowns. The soil moisture curve relates capillary pressure or pressure head with saturation as mentioned in subsection 3.1.2.. Hence, we can use the unsaturated flow equation derived from the control volume approach with the soil moisture curve (e.g. Brooks and Corey or van Genuchten) to solve for saturation and pressure head.

The control volume approach involves conducting a mass balance for fluid flow on a certain volume or grid block. As shown in Fig. (3.9), for any block, the mass balance is as follows,

$$Accumulation = Mass\ in - Mass\ out \quad (3.16)$$

where the accumulation term can be expressed as,

$$Accumulation = \left(\frac{\rho_w \phi_i}{\Delta t} \cdot (S_{w,i}^{t+\Delta t} - S_{w,i}^t) \right) \Delta x \Delta y \Delta z \quad (3.17)$$

where ρ_w is the water density, ϕ_i is the porosity at block i, Δt is the size of time step, Δx , Δy and Δz are the size of the grid blocks in the x, y and z directions, respectively.

Since the code is one dimensional, the values of Δx and Δy are assumed to be unity and Δz is the size of the grid block in the vertical direction which is assumed constant for this code.

The porosity ϕ_i is assumed constant throughout the column. $S_{w,i}^{t+\Delta t}$ and $S_{w,i}^t$ are the water saturations of the i^{th} block at times $t+\Delta t$ and t , respectively.

As discussed in subsection 3.1.4, the mass flux can be calculated from Darcy Law for unsaturated flow (Eq. (3.10)). The equation for the mass in and out can be written as follows,

$$\text{Mass in} = \rho_w K(\theta)_{i+1/2} \cdot \left(\frac{h_{w,i+1} - h_{w,i}}{\Delta z} \right) \quad (3.18)$$

$$\text{Mass out} = \rho_w K(\theta)_{i-1/2} \cdot \left(\frac{h_{w,i} - h_{w,i-1}}{\Delta z} \right) \quad (3.19)$$

where $K(\theta)_{i\pm 1/2}$ is the unsaturated hydraulic conductivity, $i+1/2$ and $i-1/2$ indicate the grid block interface as shown in Fig. (3.9) and h_w is the hydraulic head.

Figure 3.9- General layout for the modelled column

Haverkamp and Vauclin (1979) investigated different ways to calculate the unsaturated hydraulic conductivity at the interface between blocks. They found that when,

$$K(\theta)_{i\pm 1/2} = (K(\theta)_i \cdot K(\theta)_{i\pm 1})^{1/2} \quad (3.20)$$

the associated error from the geometric mean of the surrounding blocks is minimal.

Therefore, Eq. (3.20) was used to calculate $K(\theta)$ at the interfaces.

3.2.2.2 BOUNDARY AND INITIAL CONDITIONS

When a numerical technique is used to solve the flow equation, as the finite difference technique used in this code, boundary and initial conditions have to be assigned before starting the solution (i.e. at $t = 0.0$). The initial condition in this case is the values of the total head at each grid block. The total head values must be assigned a specified value as,

$$h_w(z) = h_{w,i} \quad \text{from } z = 0 \text{ to } z = L, t = 0 \quad (3.21)$$

where L is the column length.

For the boundary conditions (BCs), two different types of boundary conditions are implemented in the code; Dirichlet BC (Type 1 BC or specified total head) and Neuman BC (Type 2 BC or specified flux). One of these two boundary conditions must be assigned for the first and last grid blocks (block number 1 and block number n). In addition, the code allows the user to specify a flux for any block.

Also, it should be noted that for the assigned flux values, a positive value indicates a source term and negative value indicates a sink term. The flux boundary condition is considered as a source/sink term in the flow equation.

The boundary conditions can be written in equation form as follows,

$$h_w = h_{w,l} \quad \text{or } q = q_l \quad \text{for } z = 0 \text{ and } t \geq 0 \quad (3.22)$$

$$h_w = h_{w,n} \quad \text{or } q = q_n \quad \text{for } z = L \text{ and } t \geq 0 \quad (3.23)$$

Also, the code can solve for different stress periods where the values for the total heads and fluxes at any grid block can be changed from one stress period to the next. The user has the ability to specify the number of the stress periods and the appropriate boundary conditions for each stress period.

3.2.2.3 METHOD OF SOLVING THE FLOW EQUATION

The general flow equation in the unsaturated soil zone can be written as follows:

$$\frac{\partial(\phi S_w)}{\partial t} = \frac{\partial}{\partial z} \left(K(S_w) \frac{\partial h_w}{\partial z} \right) \pm q \quad (3.24)$$

The above flow equation is a nonlinear partial differential equation and hence a numerical method has to be used to solve the system of equations that have been generated. The Newton-Raphson technique is used to solve the system of equations in this code. The tri-diagonal matrix associated with the solution is solved using the Thomas algorithm at each time step. Further explanation and details on the Newton-Raphson technique and the solution of the Thomas algorithm are provided in Appendix A.

3.2.3 CONTAMINANT TRANSPORT EQUATION AND METHOD OF SOLUTION

3.2.3.1 CONTAMINANT TRANSPORT EQUATION

According to Baek et al. (1989), the contaminant transport equation in the unsaturated zone with a source/sink term is as follows,

$$\frac{\partial(\phi S_w C)}{\partial t} = \frac{\partial}{\partial z} \left(\phi S_w D_s \frac{\partial C}{\partial z} \right) - \frac{\partial(qC)}{\partial z} - \phi S_w R_s \quad (3.25)$$

where C is the concentration of the substrate (mg/L), D_s is the dispersion coefficient (cm^2/s) and R_s is the source/sink term which will be discussed in detail in the following subsections.

3.2.3.2 ADVECTION

Advection is the transport of solute by the groundwater flow. The flow velocity, V , (i.e. the seepage velocity) can be obtained as described in Eq. (3.9). The one-dimensional mass flux due to advection, F , will be as follows:

$$F = V n_e C \quad (3.26)$$

The change in the mass of the contaminant over time in the control volume will be,

$$n_e S_w \frac{\partial C}{\partial t} dx dy dz \quad (3.27)$$

Conservation of mass states the inflow mass minus the outflow mass equals the accumulation or change in storage which gives,

$$F - \left(F + \frac{\partial F}{\partial z} dz \right) = - \frac{\partial F}{\partial z} dz = - n_e \frac{\partial}{\partial z} (V C) dz \quad (3.28)$$

Hence, for homogeneous aquifer, the one-dimensional advection transport equation is:

$$\frac{\partial(S_w C)}{\partial t} = - \frac{\partial(V C)}{\partial z} \quad (3.29)$$

3.2.3.3 DIFFUSION

Diffusion is the flux of solute from a zone of higher concentration to a zone of lower concentration. For the steady state case, this process is described by Fick's law as,

$$F = -D_{AB} \frac{\partial(\phi.S_w.C)}{\partial z} \quad (3.30)$$

where D_{AB} is the diffusion coefficient. It was suggested to use an effective diffusion coefficient $D^* = \tau D_{AB}$, with τ ranging from 0.01 to 0.5, to take into account the tortuosity of the flow paths in porous media (Delleur 1999).

Thus, using Fick's second law, the change in concentration over time inside a control volume subjected to diffusion flux can be determined by,

$$\frac{\partial C}{\partial t} = D^* \frac{\partial^2 C}{\partial z^2} \quad (3.31)$$

3.2.3.4 DISPERSION

Dispersion is the measure of how a contaminant will spread along and across the main flow direction due to velocity variations and aquifer heterogeneities at both pore and regional scale.

If one considers a representative elementary volume (REV), dispersion can be described by Fick's law. The dispersion coefficient, D_s includes the effect of diffusion

and dispersion. The dispersion coefficient can be introduced in the longitudinal and the transverse direction as follows,

$$D_L = \alpha_L V + \tau D_{AB} \quad (3.32)$$

and,

$$D_T = \alpha_T V + \tau D_{AB} \quad (3.33)$$

where α is the dispersivity, τ is the tortuosity, L and T are longitudinal and the transverse directions respectively (Delleur 1999).

3.2.3.5 NUMERICAL SOLUTION

In the proposed code, the contaminant transport equation is solved using the finite difference technique. To solve the equation using finite difference, the domain has to be divided into a series of vertical grid blocks. As per the flow equation, the code assumes the domain is divided into equal size grid blocks. Fig. (3.10) shows layout of three grid blocks equally divided. The concentration is assigned at the center of each block.

Due to the well known problems dealing with the contaminant transport problems with a sharp front, two spatial weighting schemes were considered; the upstream and central weighting. Upstream weighting is used at the beginning of the simulation to handle the sharp front problem. At later times central weighting or upstream weighting can be used to continue the simulation. The user has the flexibility to select the upstream or central weighing for each assigned stress period.

Figure 3.10- Block-centered finite difference discretization of a one-dimensional problem domain (Zheng and Bennett 1995).

For more details of how the central and upstream weighting schemes were derived, the reader should refer to Appendix A. It should be noted that the finite difference approach is based on the control volume approach and the mass balance for the advection and dispersion terms are provided in Appendix A.

After setting up the finite difference equation, a numerical scheme is needed to solve for the unknowns, which are the concentration values in this case. Two schemes can be used to solve this type of problems; explicit scheme and implicit scheme.

The proposed model solves the equations using an explicit scheme. In the explicit scheme, we are seeking $C_i^{t+\Delta t}$ with the knowledge of the concentrations at the previous time step (i.e. C_{i+1}^t , C_i^t and C_{i-1}^t , Fig. (3.11)). For the explicit scheme there is no matrix involved and the solution can be done easily. The set of equations will be in the form of,

$$C_i^{t+\Delta t} = a_1 C_{i-1}^t + a_2 C_i^t + a_3 C_{i+1}^t \quad (3.34)$$

where a_1 , a_2 and a_3 are coefficient which are defined in Appendix A.

Figure 3.11- Explicit scheme

Dealing with contaminant transport in the unsaturated zone can generate a double sharp front problem. The first sharp front is generated by an infiltration event for the flow equation. As the saturation moves in the unsaturated soil, the saturation varies almost from 100% to the irreducible saturation and this generates a numerical stability problem when solving the flow equation. Also, as mentioned previously, there is a sharp front generated by the introduction of a contaminant where at the front the concentration varies sharply from C/C_o of 1.0 to zero. Hence, it can be considered a double sharp front problem and it may generate oscillation behaviour. The upstream weighting scheme is the best solution for this problem as it gives more weight on the upstream nodes in the direction of the flow. In addition, the oscillation problem depends on the degree to which the dispersion term governs the solute transport. When the dispersion dominates, the oscillation problem disappears because the sharp front is dispersed.

3.2.3.6 BOUNDARY AND INITIAL CONDITIONS

Initial and boundary conditions have to be assigned before the simulation starts. For the initial conditions, a concentration of zero mg/L is assigned to each grid block as the initial concentration (Eq. (3.38)).

$$C = 0 \quad 0 > z \geq L, t = 0 \quad (3.35)$$

The boundary condition at the top grid block can be either a prescribed concentration, C_o , or a prescribed flux, qC_o .

For the bottom grid block, the concentration is calculated according to a control volume approach which just allows the mass to leave the grid block via advection only. Hence, the code assumes contaminant mass can enter or leave the domain at any location.

Fig. (3.12) shows graphically the approach used to calculate the concentration at the first, last and intermediate grid blocks.

Also, the code can solve for different boundary concentration values at different stress periods where the values for the C_o can be changed. The user can specify a value for C_o during one stress period and this value can be changed in the next stress period, if needed.

Figure 3.12- Graphical representation for the initial and boundary concentrations.

3.2.4 SOURCE / SINK TERMS

Two different source/sink terms were implemented in the proposed code. The user can select first order decay rate to simulate the decay of a certain contaminant or Monod kinetics to simulate the biodegradation of a certain contaminant. Further explanation for these two terms are provided in detail in the next subsections.

3.2.4.1 FIRST ORDER DECAY RATE

The first order decay rate can be expressed as follows,

$$\frac{\partial C}{\partial t} = -\lambda C \quad (3.36)$$

where C is the concentration of the contaminant of interest, λ is a decay coefficient and t is the time.

According to James et al. (1999), the coefficient λ can be calculated as follows,

$$\lambda = -\frac{\ln 2}{T_{1/2}} \quad (3.37)$$

where $T_{1/2}$ is the decay half life of the contaminant of interest.

The analytical solution for the first order decay rate can be obtained from,

$$C = C_o e^{-\lambda t} \quad (3.38)$$

When first order decay rate is the sink term chosen by the user, the contaminant transport equation will be in the form of,

$$\frac{\partial(\phi S_w C)}{\partial t} = \frac{\partial}{\partial z} \left(\phi S_w D_s \frac{\partial C}{\partial z} \right) - \frac{\partial(q C)}{\partial z} - \phi S_w \lambda C \quad (3.39)$$

where R_s in Eq. (3.25) is substituted by (λC) to take into account the first order decay rate as a sink term.

3.2.4.2 MONOD KINETICS

Monod kinetics is the model chosen to simulate the biodegradation of a certain contaminant and the corresponding growth and decay of the microbial mass. In considering Monod kinetics, the source/sink term in the one-dimensional advection-dispersion equation (R_s) can be calculated as follows,

$$\frac{\partial C}{\partial t} = -R_s = -(M_T)(q_m) \left(\frac{C}{K_s + C} \right) \quad (3.40)$$

and the complete one-dimensional transport equation can be written as:,

$$\frac{\partial(\phi S_w C)}{\partial t} = \frac{\partial}{\partial z} \left(\phi S_w D_s \frac{\partial C}{\partial z} \right) - \frac{\partial(q C)}{\partial z} - (\phi)(S_w)(M_T)(q_m) \left(\frac{C}{K_s + C} \right) \quad (3.41)$$

where, M_T is the microbial concentration (mg/L), q_m is the maximum specific rate of substrate utilization (mg substrate / mg cell . s), K_s is the half-velocity constant (mg/L) and C is the substrate concentration as mentioned before (mg/L).

The change in microbial concentration with time can be calculated as follows,

$$\overbrace{\frac{\partial M_T}{\partial t}}^{\text{Change in microbial concentraion with time}} = \overbrace{(Y)(M_T)(q_m)\left(\frac{C}{K_s + C}\right)}^{\text{Growth rate}} - \overbrace{(b)(M_T)}^{\text{Decay rate}} \quad (3.42)$$

where, Y is the cell yield coefficient (mg cell / mg substrate) and b is the cell decay coefficient (s^{-1}).

3.2.4.2.1 SOLUTION PROCEDURE

It should be noted that the contaminant transport equation is a partial differential equation and it is function of two unknowns, the concentration of the substrate (C) and the microbial concentration (M_T) which are varying with time. Also, Eq. (3.42) is an ordinary differential equation function of one unknown which is the microbial concentration.

Fig. (3.13) shows how the contaminant transport and the microbial growth and decay equations are organized simultaneously to solve for the contaminant and microbial concentrations at each time step.

Figure 3.13- Flow chart shows solution sequence of the contaminant and the microbial equations.

As shown in Fig. (3.13), the initial concentrations are used as an initial value to determine microbial concentration (M_T) (Eq. (3.42)). After obtaining M_T , source/sink term (R_S) is calculated based on the concentration values and M_T (Eq. (3.40)). Then R_S is substituted into the advection dispersion equation (Eq. (3.41)) which is solved explicitly.

3.2.4.2.2 OPERATOR-SPLITTING AND RUNGE-KUTTA METHOD TO SOLVE ORDINARY DIFFERENTIAL EQUATIONS

Eq. (3.25) is a complicated equation to be solved in one step as shown in the previous subsection. Operator-splitting is the approach used to solve for the substrate concentration and the microbial concentrations. Using operator splitting, one can divide the solution of the equation into two parts, solving the advection-dispersion part first (Eq. (3.43)) then solve for the reaction or biodegradation part (Eq. (3.44)) as follows,

$$\frac{\partial(\phi S_w C)}{\partial t} = \frac{\partial}{\partial z} \left(\phi S_w D_s \frac{\partial C}{\partial z} \right) - \frac{\partial(qC)}{\partial z} \quad (3.43)$$

$$\frac{\partial(\phi S_w C)}{\partial t} = -\phi S_w R_s \quad (3.44)$$

where R_s represents the reaction of interest. This decoupling is an efficient way to deal with complex reactions where the reaction time maybe much smaller than the advection – dispersion time step. Fig. (3.14) shows graphically one operator-split cycle as shown by Odencrantz et al. (1990).

Figure 3.14- Graphical representation of one complete operator- split cycle (Odencrantz et al. 1990).

After splitting the contaminant transport equation into advection–dispersion and biodegradation components, a method is needed to solve system of nonlinear ordinary differential equations for the biodegradation equation (Eq. (3.44)). The Runge-Kutta method is the technique used to solve system of nonlinear ordinary differential equations (Dennis and Schnabel 1983; Odencrantz et al. 1990). A fourth-order Runge-Kutta method is used because it is fifth order accurate in time (Dennis and Schnabel 1983; Odencrantz et al. 1990). Further mathematical explanation of Runge-Kutta method can be found in Appendix A.

3.2.4.2.3 CONVERTING FROM MICROBIAL CONCENTRATION TO SATURATION

This subsection illustrates the procedures used to convert from concentration of microbes to microbial saturation, which is a term used to develop the conceptual model for unsaturated clogging.

The user must prescribe a constant initial microbial concentration over the entire domain. The mass of microbes within a grid block can be obtained as follows,

$$\text{Microbial Mass} = \overbrace{\bar{M}_T}^{\text{Concentration}} \overbrace{\Delta x \Delta y \Delta z \phi S_w}^{\text{Saturated Voids}} \quad (3.45)$$

and the microbial mass can be converted into a microbial volume using,

$$\text{Microbial Volume} = \frac{\text{Microbial Mass}}{\rho_{\text{dry bacteria}}} \quad (3.46)$$

The actual saturation of the microbes can be calculated as follows,

$$S_{am} = \frac{\text{Microbial Volume}}{\text{Void Volume}} \quad (3.47)$$

and the effective microbial saturation as,

$$S_{em} = \frac{S_{am}}{\left(1 - \frac{\theta_r}{\phi}\right)} \quad (3.48)$$

3.2.5 MASS BALANCE

A mass balance calculation is one of the most important tools used to check that a code is functioning properly. In the proposed code, a mass balance function was developed to check that the flow equation and the contaminant transport equation are conserving mass.

3.2.5.1 FLUID MASS BALANCE

To implement a mass balance to check whether the flow equation is coded correctly, the resultant mass balance for the entire model domain at each time step has to be calculated as follows,

$$\text{Mass Balance at a certain time step} = \text{In flow} - \text{Change in storage} - \text{Out flow} \quad (3.49)$$

seeking a value of zero for the left hand side.

The “In flow” includes all the fluid mass flux terms entering the model domain. If the top boundary is a type 2 BC or flux boundary, the “In flow” value can be calculated as follows,

$$\text{In flow} = \text{Flux at the boundary} \cdot \Delta t + \sum [(Flux In)_i \Delta t] \quad (3.50)$$

where i represents the block number. It should be noted that the code allows the user to add flux at any grid block as mentioned in the previous subsections.

If the top boundary condition is type 1 BC or prescribed head, then the “In flow” can be calculated as follows,

$$\text{In flow} = k_r K_{sat} \Delta t \left(\frac{h_{(at the top boundary)} - h_{(last grid block - 1)}}{\Delta z} \right) + \sum [(Flux In)_i \Delta t] \quad (3.51)$$

For the “Out flow”, in case of type 2 BC, the value can be calculated as follows,

$$\text{Out flow} = \text{Flux at the boundary} \Delta t + \sum [(Flux Out)_i \Delta t] \quad (3.52)$$

and if type 1 BC is used, the value can be calculated using,

$$Out\ flow = k_r\ K_{sat}\ \Delta t \cdot \left(\frac{h_{(at\ the\ first\ grid\ block)} - h_{(at\ the\ bottom\ boundary)}}{\Delta z} \right) + \sum [(Flux\ In)_i\ \Delta t] \quad (3.53)$$

The accumulation term is calculated by subtracting the saturation profile at a certain time step from the saturation profile at the previous time step where,

$$Area\ under\ the\ curve\ at\ time\ (t + \Delta t) = \sum_{i=1}^n [S_w(t + \Delta t)\ \Delta z\ \phi] \quad (3.54)$$

$$Area\ under\ the\ curve\ at\ time\ (t) = \sum_{i=1}^n [S_w(t)\ \Delta z\ \phi] \quad (3.55)$$

and,

$$\begin{aligned} Change\ in\ storage\ at\ time\ (t + \Delta t) &= Area\ under\ the\ curve\ at\ time\ (t + \Delta t) \\ &\quad - Area\ under\ the\ curve\ at\ time\ (t) \end{aligned} \quad (3.56)$$

The cumulative flow mass balance can be calculated by summing the inflow, outflow and changes in storage for all time steps.

3.2.5.2 CONTAMINANT MASS BALANCE

Using the same concept used for the flow equation mass balance, a contaminant mass balance is implemented to check whether the contaminant transport equation is implemented properly. The resultant mass balance at each time step has to be calculated as follows,

$$\begin{aligned} Mass\ Balance\ at\ a\ certain\ time\ step &= Contaminant\ mass\ In - Accumulation - \\ &\quad Degradation - Contaminant\ mass\ Out \end{aligned} \quad (3.57)$$

seeking a value of zero for the left hand side.

If a type 2 BC is applied at the top boundary, then the “Contaminant mass In” value can be calculated as follows,

$$\text{Contaminant mass In} = \text{Flux at the boundary} \Delta t C + \sum [(Flux In)_i \Delta t C_{o_i}] \quad (3.58)$$

where C is the concentration and i represents the block number.

If the top boundary condition is type 1 BC, then the “Contaminant mass In” can be calculated as follows,

$$\begin{aligned} \text{Contaminant mass In} = C k_r K_{sat} \Delta t \left(\frac{h_{(at the top boundary)} - h_{(last grid block-1)}}{\Delta z} \right) \\ + \sum [(Flux In)_i \Delta t C_{o_i}] \end{aligned} \quad (3.59)$$

If the lower boundary is a type 1 BC, the “Contaminant mass Out” value can be calculated as follows,

$$\text{Contaminant mass Out} = \text{Flux at the boundary} \Delta t C + \sum [(Flux Out)_i \Delta t C_i] \quad (3.60)$$

and if it is type 2 BC, the value can be calculated using,

$$\begin{aligned} \text{Contaminant mass Out} = C k_r K_{sat} \Delta t \left(\frac{h_{(at the first grid block)} - h_{(at the bottom boundary)}}{\Delta z} \right) \\ + \sum [(Flux Out)_i \Delta t C_i] \end{aligned} \quad (3.61)$$

The accumulation term is calculated by subtracting the contaminant mass in the domain at a certain time step from the contaminant mass in the domain at the previous time step where,

Mass in the domain at time $(t + \Delta t) =$

$$\left[\sum_{i=1}^n \text{Concentration profile at time } (t + \Delta t) (S_w) \Delta z \phi \right] \quad (3.62)$$

$$\text{Mass in the domain at time } (t) = \sum_{i=1}^n [\text{Concentration at time } (t) (S_w) \Delta z \phi] \quad (3.63)$$

and,

$$\begin{aligned} \text{Accumulation at time } (t + \Delta t) &= \text{Mass in the domain at time } (t + \Delta t) \\ &\quad - \text{Mass in the domain at time } (t) \end{aligned} \quad (3.64)$$

If first order decay rate is used as a sink term, the degradation during a certain time step can be calculated as follows,

$$\text{Degradation} = \lambda C \Delta z \Delta t (S_w) \phi \quad (3.65)$$

If Monod Kinetics is used as a sink term, the degradation will be calculated as follows,

$$\text{Degradation} = (M_T)(q_m) \left(\frac{C}{K_s + C} \right) (S_w)(\phi)(\Delta z)(\Delta t) \quad (3.66)$$

The cumulative contaminant mass balance can be calculated by summing the contaminant mass in, contaminant mass out, mass in the domain and degradation for all time steps.

4 THE PROPOSED CONCEPTUAL MODELS FOR RELATIVE PERMEABILITY

4.1 INTRODUCTION

Three conceptual models for bioclogging in unsaturated soils were proposed and implemented in the one dimensional C++ code in order to simulate the impact of the bacteria growth on flow in the unsaturated zone. The proposed conceptual models varied in approach from macroscopic to microscopic and varied in form from analytical to empirical.

4.2 MODEL #1

As discussed early in the previous chapter, the voids in the unsaturated soil can be simulated as capillary tubes with different diameters; each diameter reflects a volume of void space that can be filled at a certain capillary pressure. Under unsaturated conditions, the smaller pores contribute to fluid flow. Since the biodegradable substrate will be in these smaller pores, one could assume that the microbial growth will occur in the smaller pores. Hence, when bacteria start to grow, the small diameter pores will be clogged first by the bacteria cells and the relative permeability will be reduced to compensate for the clogging of the smaller pores. As a result, the water content will increase to allow a corresponding increase in the relative permeability to conduct the same fluid flow and the flow will be displaced into the larger pores. Meanwhile, the bacteria in the larger pores will be in contact with nutrients and food and they will continue growing and displacing the flow to the larger pores. This process will take place until all the pores contain

bacteria cells and no more water can be conducted in the pores. Hence, the soil will be fully clogged (Fig. (4.1)).

Based on the formulations put forward by Burdine (1953) and Mualem (1976) to estimate the relative permeability term, Lenhard and Parker (1987) proposed relative permeability terms for two-phase flow systems (e.g. water and air or non-aqueous phase liquid (NAPL) with fluid entrapment) and three-phase flow systems (water, NAPL and air). For example, for a water-air system with air entrapment, they assumed that *“the presence of immobile air bubbles occluded by the water phase will result in an obstruction to water flow. Simultaneously, trapped air will displace water into larger pores which will tend to increase the water relative permeability at a given actual water saturation above that which would occur in the absence of air entrapment”*. To account for these effects they modified Mualem’s equation (Eq. (3.15)) to account for the impact of the entrapped air on the relative permeability of the water phase (k_{rw}). They modified Eq. (3.15) as follows:

$$k_{rw}(S_{aw}) = S_{aw}^{1/2} \left(\frac{\int_0^{S_{aw}} \frac{dS_{aw}}{\psi} - \int_0^{S_{trap}} \frac{dS_{trap}}{\psi}}{\int_0^1 \frac{dS_{aw}}{\psi}} \right)^2 \quad (4.1)$$

where they called S_{aw} the apparent water saturation and S_{trap} the effective entrapped air saturation.

A similar approach was used here to account for microbial growth. In Fig. (4.2), S_{em} is the effective microbial saturation, S_{ew} is the effective water saturation and S_{et} is the effective total saturation.

Figure 4.1- Visualization of Model #1

Figure 4.2- Capillary pressure – saturation relationship for Model #1

The integral form from Burdine (1953) or Mualem (1976) can be altered to reflect the presence of a microbial saturation as follows:

$$\text{For Burdine} \quad k_r(S_{ew}) = S_{et}^2 \frac{\int_0^{S_{et}} \frac{dS_e}{\psi^2} - \int_0^{S_{em}} \frac{dS_e}{\psi^2}}{\int_{S_e=0}^1 \frac{dS_e}{\psi^2}} \quad (4.2)$$

$$\text{For Mualem} \quad k_r(S_{ew}) = S_{et}^{1/2} \left(\frac{\int_0^{S_{et}} \frac{dS_e}{\psi} - \int_0^{S_{em}} \frac{dS_e}{\psi}}{\int_{S_e=0}^1 \frac{dS_e}{\psi}} \right)^2 \quad (4.3)$$

Eq. (4.2) using Burdine's theory and Eq. (4.3) using Mualem's theory, express the relation between the relative permeability and the saturation taking into account the microbial growth where the additional term $\int_0^{S_{em}} \frac{dS_e}{\psi^2}$ for Burdine and $\int_0^{S_{em}} \frac{dS_e}{\psi}$ for Mualem is to take into account the effect of bacterial growth on the relative permeability term.

The closed form of the integral equations (4.2) and (4.3) are given as:

$$\text{Burdine} \quad k_r(S_{ew}) = S_{et}^2 \left((1 - S_{em}^{1/m})^m - (1 - S_{et}^{1/m})^m \right) \quad (4.4)$$

$$\text{Mualem} \quad k_r(S_{ew}) = S_{et}^{1/2} \left((1 - S_{em}^{1/m})^m - (1 - S_{et}^{1/m})^m \right)^2 \quad (4.5)$$

4.3 MODEL #2

In the second model, the original integration developed by Burdine and Mualem is used (Fig. (4.3)).

The relationship between the saturation and the relative permeability as a function of the effective water saturation will be multiplied by a new term, $(1 - S_{em})$, to reduce the

relative permeability term by a factor to take into account the impact of microbial growth on relative permeability.

Figure 4.3- Capillary pressure – saturation relationship for Model #2

The equations used for Model #2 based on Burdine and Mualem are as follows:

For Burdine
$$k_r(S_{ew}) = S_{ew}^2 \left(1 - \left(1 - S_{ew}^{1/m} \right)^m \right) \cdot (1 - S_{em}) \quad (4.6)$$

For Mualem
$$k_r(S_{ew}) = S_{ew}^{1/2} \left(1 - \left(1 - S_{ew}^{1/m} \right)^m \right)^2 \cdot (1 - S_{em}) \quad (4.7)$$

There is no experimental proof or theoretical derivation for this formulation. The second model provides a quick estimation of the relative permeability term. It assumes that the bacteria will grow in the smaller pores first and with time flow is displaced to the larger pores, as was proposed in the first model. Further experimental work needs to be done to confirm whether this second conceptual scenario is valid or not.

4.4 MODEL #3

The third model is based on a microscale conceptual model. As discussed in the previous chapter, the unsaturated soil can be considered as a series of capillary tubes with different diameters. Eq. (3.1) relates the capillary pressure in these tubes with the radius of the capillary tubes. For unsaturated flow, the soil moisture curve is known and the pore size distribution can be inferred from this capillary pressure-saturation relationship. In this proposed conceptual model, the pore distribution is determined or inferred from the soil moisture curve and the microbial growth is assumed to form a biofilm that covers the walls of the capillary tubes. For the third model, the biofilm is assumed to form in all the pores since all the pores contain an irreducible water saturation in which the bacteria can grow. The reduction in the radii of the capillary tubes will increase the resistance to flow and reduce the permeability of those pores. Based on these assumptions, this model was developed. A conceptual schematic of the model is provided in Fig. (4.4).

In developing this conceptual model, the capillary pressure-saturation relationship will be used to determine pore size distribution. The van Genuchten relationship (i.e. Eq. (3.13)) is the relationship used in the code and can be rearranged to solve for capillary pressure. The resulting equation is as follows:

$$\psi = \frac{\left(S_e^{\frac{-1}{m}} - 1 \right)^{\frac{1}{n}}}{\alpha} \quad (4.8)$$

To determine the distribution of radii for the bundle of capillary tubes representing the soil, the saturation is divided into a user-specified number of equal divisions. The average saturation at the midpoint of each division is then used to

determine the corresponding capillary pressure. The capillary pressure is used to calculate the radius of the capillary tube.

Figure 4.4- Visualization of Model #3

Fig. (4.5) gives an example of how a 4-division scenario is evaluated. The saturations at the mid points of each division will be 0.125, 0.375, 0.625 and 0.875. Using these saturations, the capillary pressures values P_{c1} , P_{c2} , P_{c3} and P_{c4} can be calculated. Knowing the surface tension of the water/air interface, the corresponding radii can be calculated using Eq.(3.1).

Figure 4.5- Example of choosing 4 radii of capillary tubes

Each division represents an equal fraction of the saturation or an equal fraction of a void volume. For the previous simple example, each radius represents a group of capillary tubes representing 25% of the saturation. Essentially, the domain's void volume is divided into 4 divisions, each division has the same void volume (Fig. (4.6)).

The number of capillary tubes within each division can be calculated by dividing the total void volume of each division (represented as a cross section area) by the cross-sectional area of one capillary tube.

Once the distribution of capillary tubes is known, the microbial volume can then be distributed as a biofilm of uniform thickness, th , within the capillary tubes using the following equation:

$$\sum_{i=1}^{\# \text{ of divisions}} \left(\# \text{ of Tubes}_i \cdot \pi \cdot r_i^2 - \# \text{ of Tubes}_i \cdot \pi \cdot (r_i - th)^2 \right) = V_m \quad (4.9)$$

Figure 4.6- Domain is divided into 4 sections each have the same void volume.

Based on Hagen Poiseuille's derivation for laminar flow in a pipe and summing the flows within all the capillary tubes, a total flow can be estimated using the following equation:

$$Q = - \frac{\sum_{i=1}^{\# \text{ of divisions}} (\# \text{ of Tubes})_i \pi r_i^4}{8} \frac{\rho g}{\mu} \frac{\partial h}{\partial L} \quad (4.10)$$

as,

$$K(\theta) = K_{sat} k_r \cong \left(\frac{\sum_{i=1}^{\# \text{ of divisions}} (\# \text{ of Tubes})_i \pi r_i^4}{8} \frac{\rho g}{\mu} \right) (k_r) \quad (4.11)$$

where r is the radius of the capillary tube, ρ is the density of the liquid, g is the gravitational acceleration, μ is the dynamic viscosity.

The presence of a biofilm will impact this flow and Eq. (4.10) could be modified as follows:

$$Q = - \frac{\sum_{i=1}^{\# \text{ of divisions}} (\# \text{ of Tubes})_i \pi (r_i - th)^4}{8} \frac{\rho g}{\mu} \frac{\partial h}{\partial L} \quad (4.12)$$

where th is the thickness of the biofilm layer.

Hence, to adjust the unsaturated permeability of the soil to account for the impact of the biofilm, a flow factor, U , is introduced and the ratio of the flow factors with and without the biofilm is used to reduce the relative permeability. The flow factor without the biofilm is expressed as:

$$U_o|_0^{Porosity} = \left(- \frac{\sum_{i=1}^{\# \text{ of divisions}} (\# \text{ of Tubes})_i \pi r_i^4}{8} \frac{\rho g}{\mu} \right) \quad (4.13)$$

and with the biofilm, the flow factor is expressed as:

$$U_i|_0^{Porosity} = \left(- \frac{\sum_{i=1}^{\# \text{ of divisions}} (\# \text{ of Tubes})_i \pi (r_i - th)^4}{8} \frac{\rho g}{\mu} \right) \quad (4.14)$$

where $U_o|_0^{Porosity}$ represents the initial flow without a biofilm for all the pores (i.e. zero through porosity) and $U_i|_0^{Porosity}$ represents the reduced flow with a biofilm present in all the pores. The relative permeability term can then be reduced by a factor of $U_i|_0^{Porosity}$ over $U_o|_0^{Porosity}$.

Finally, the relative permeability saturation relationships that can be used to simulate this scenario for Burdine and Mualem are as follows:

$$\text{For Burdine} \quad k_r(S_{ew}) = S_{ew}^2 \left(1 - (1 - S_{ew}^{1/m})^m \right) \cdot \left(\frac{U_i|_0^{\text{Porosity}}}{U_o|_0^{\text{Porosity}}} \right) \quad (4.15)$$

$$\text{For Mualem} \quad k_r(S_{ew}) = S_{ew}^{1/2} \left(1 - (1 - S_{ew}^{1/m})^m \right)^2 \cdot \left(\frac{U_i|_0^{\text{Porosity}}}{U_o|_0^{\text{Porosity}}} \right) \quad (4.16)$$

Reader should note that at each time step, as the biofilm grows, the biofilm thickness increases. At a certain point, as shown in Fig. (4.4), some radii will be filled by the bacteria and will no longer contribute to the flow. As a result, Eq. (4.9) is modified with time to account for the capillary tubes which are filled.

4.5 COMPARISON BETWEEN THE REDUCTION IN THE RELATIVE PERMEABILITY SIMULATED WITH THE THREE PROPOSED MODELS

In this subsection, a comparison between the three proposed conceptual models is given to illustrate the impact of the microbial growth on the relative permeability term.

Before introducing the example that shows the comparison between the models, the reader should know that the van Genuchten parameter (n) plays an important role in the relative permeability relationship and hence will affect the clogging process.

Let us assume hypothetically that Fig. (4.7) represents the capillary pressure-saturation relationship for two different soils with the same porosity. One soil reflects a well graded soil with low n value (e.g. n = 1.3), and the second soil reflects well sorted

soil with high n value (e.g. $n = 3.0$). For a given microbial volume for both soils, assume that the smaller pore in the first soil will clog (as shown in the Fig. (4.7)) and the rest of the microbial volume will be distributed with a certain thickness which is equal or larger than the radius of the smaller pore. In the second soil, the microbial volume is distributed equally over all the pores.

Figure 4.7- Capillary pressure - relationship for two soils, well graded soil with $n = 1.3$ and well sorted soil with $n = 3.0$

If one looks at the flow through both soils using the Hagen Poisseuille equation and compares the reduction in the flow in both soils for a given microbial volume, a larger reduction in the flow will occur in the second soil versus the first one. This is due to the fact that the flow in the first soil is dominated by the largest pore. Hence, the

reduction in flow due to clogging of the smaller pores and the small reduction in radius of the larger pore is minimal. For the second soil the pores are uniform in size and are smaller than the largest pore for soil one. As a result, all the pores contribute to the flow and the microbial volume will reduce the flow in all the pores. Hence, the impact of microbial volume is greater. As a conclusion, a soil with a high van Genuchten n value will have greater reduction in the flow factor used in Model #3 versus a soil with low van Genuchten n value.

In the following example, for a peat soil, two saturation scenarios are considered for two soils with different van Genuchten n values of 1.3 and 3.0. The effective total saturation and effective microbial saturation were assumed to be 0.8 and 0.2, respectively for the first scenario and 0.8 and 0.6, respectively for the second scenario. Table (4.1) shows the data needed for Models #1, #2 and #3. Tables (4.2) and (4.3) present the two saturation scenarios for the soil with a van Genuchten n value of 1.3 and Tables (4.4) and (4.5) present the two saturation scenarios for the soil with the van Genuchten n value of 3.0. The reader should note that the values presented in the tables (i.e. Table (4.2), (4.3), (4.4) and (4.5)) do not represent real simulations and they are just to give a conceptual idea of the relationship between the models.

Table 4.1- Data needed for Models #1, #2 and #3

<i>Parameter</i>		<i>Value</i>	<i>Units</i>	<i>Parameter</i>	<i>Value</i>	<i>Units</i>
θ_r		0.08736	-----	σ	72.4	dyne/cm
K_{sat}		0.079	cm/s	μ	0.001	Pascal.s
ϕ		0.8	-----	γ	9810	N/m ³
van Genuchten	α	0.18	cm ⁻¹	Number of divisions in the P_c – Saturation curve		4
	n	1.3 & 3.0	-----			

Table 4.2 Comparison of the relative permeability reduction between the three proposed models for effective microbial saturation of 0.2 using van Genuchten n value of 1.3

S_{et} and S_{em} values	Method Used Model#	k_r values		Values of the reduction factors
		Burdine	Mualem	
$S_{et} = 0.8$ and $S_{em} = 0.2$	1	<i>For n less than 2, m becomes negative and hence Burdine's model is not applicable</i>	9.73×10^{-03}	-----
	2		4.31×10^{-04}	0.80
	3		5.37×10^{-04}	0.997
$S_{et} = 0.8$ and $S_{em} = 0.0$	Original values		9.77×10^{-03}	-----

Table 4.3 Comparison of the relative permeability reduction between the three proposed models for effective microbial saturation of 0.6 using van Genuchten n value of 1.3

S_{et} and S_{em} values	Method Used Model#	k_r values		Values of the reduction factors
		Burdine	Mualem	
$S_{et} = 0.8$ and $S_{em} = 0.6$	1	<i>For n less than 2, m becomes negative and hence Burdine's model is not applicable</i>	5.47×10^{-03}	-----
	2		8.35×10^{-09}	0.40
	3		1.78×10^{-08}	0.85
$S_{et} = 0.8$ and $S_{em} = 0.0$	Original values		9.77×10^{-03}	-----

Table 4.4- Comparison of the relative permeability reduction between the three proposed models for effective microbial saturation of 0.2 using van Genuchten n value of 3.0

S_{et} and S_{em} values	<i>Method Used Model#</i>	k_r values		Values of the reduction factors
		Burdine	Mualem	
S_{et} = 0.8 and S_{em} = 0.2	1	1.34×10^{-01}	2.30×10^{-01}	-----
	2	2.24×10^{-02}	7.20×10^{-02}	0.80
	3	2.18×10^{-02}	7.00×10^{-02}	0.77
S_{et} = 0.8 and S_{em} = 0.0	Original values	1.36×10^{-01}	2.88×10^{-01}	-----

Table 4.5- Comparison of the relative permeability reduction between the three proposed models for effective microbial saturation of 0.6 using van Genuchten n value of 3.0

S_{et} and S_{em} values	<i>Method Used Model#</i>	k_r values		Values of the reduction factors
		Burdine	Mualem	
S_{et} = 0.8 and S_{em} = 0.6	1	8.63×10^{-02}	4.60×10^{-02}	-----
	2	4.28×10^{-05}	6.56×10^{-04}	0.40
	3	4.04×10^{-05}	6.20×10^{-04}	0.378
S_{et} = 0.8 and S_{em} = 0.0	Original values	1.36×10^{-01}	2.88×10^{-01}	-----

The 5th column in Tables (4.2), (4.3), (4.4) and (4.5) presents the values of the reduction factors (i.e. $(1 - S_{em})$ factor for Model #2 and the flow factor for Model #3). A spread sheet file used in the calculations of the relative permeability values given in Tables (4.4) and (4.5) is described in Appendix (A).

As described earlier in this Chapter, Model #1 assumes that the smaller pores will fill first with microbes, and at lower microbial saturation values, only the smaller pores will be filled with microbes. Since the smaller pores contribute least to the flow, Model #1 should predict the lowest reduction on the relative permeability as shown in Tables (4.2) through (4.5). For an effective microbial saturation of 0.2, a slight reduction occurs in the relative permeability (e.g. reduced from 9.77×10^{-3} to 9.73×10^{-3} for the soil with $n = 1.3$; Table (4.2)). For an effective microbial saturation of 0.6, the impact is larger, however, for Model #1 the relative permeability is reduced by less than 50% in comparison to the relative permeability values without microbial growth.

On the other hand, Model #2 predicts higher reduction in the relative permeability value in comparison to Model #1. As discussed earlier, the relative permeability will be reduced by a factor of $(1 - S_{em})$ which reduces the relative permeability by 20% for the first saturation scenario with $S_{em} = 0.2$. In addition, the effective water saturation term in Burdine's and Mualem's equation is reduced. Therefore, a significant reduction in the relative permeability value will be calculated for Model #2 for a $S_{em} = 0.2$. Model #3 indicates a similar impact on the relative permeability term. The reader is referred to Chapter 5 for additional plots that show a reduction in the flow factor (Model #3) and the $(1 - S_{em})$ factor (Model #2) with time for the scenarios presented in Chapter 5.

For an effective microbial saturation of 0.6 and an effective total saturation of 0.8, the same behaviour is expected (Tables (4.3) and (4.5)). A significant reduction in the relative permeability is associated with Model #2 and Model #3 versus Model #1.

As discussed earlier in terms of the difference between van Genuchten n values, the reduction in the factors presented in the tables support the conclusion that a greater n value (well sorted soil) will result in a greater reduction in the relative permeability for a given S_{em} when compared to the reduction calculated for an n value of 3.0 (well graded soil) (i.e. flow factor of 0.378 for $n = 3.0$ and 0.85 for $n = 1.3$ for an effective microbial saturation of 0.6).

5 UNSATURATED MODEL DEVELOPMENT

5.1 INTRODUCTION

The first part of this chapter deals with verification cases for the C++ code developed as a part of this research. Different verification cases were tested to verify that the equations were coded correctly in the code. Unfortunately, due to lack of verification data in this area of research, not all the equations were verified. For this reason, conceptual cases were used to verify the equations that had no data for verification. The two main equations that need to be verified in the code are the flow equation and contaminant transport equation. The mass balance function that was described earlier in Chapter 3 is used to support that the equations are coded correctly and to provide additional support for the equations that had no verification data (e.g. unsaturated flow with Monod kinetics).

The second part in this chapter demonstrates the functionality of the code through various model simulations. Different data sets were used to generate results that compare the proposed clogging models, which link the microbial growth with the relative permeability of the soil.

5.2 CODE VERIFICATION

5.2.1 FLOW EQUATION VERIFICATION

Two different cases were used from the literature to verify the flow equation. The main difference between these two cases is that they use different boundary conditions.

5.2.1.1 CASE 1: TWO PHASE INFILTRATION

In 1986, Touma and Vauclin conduct several experiments on sandy soil columns to investigate two phase infiltration. They modeled the results measured for water content and pressure heads numerically with a one dimensional, finite difference flow code. They show that air movement significantly impacts some variables such as volumetric water content profiles and infiltration rates. The data extracted from their experimental work that have been used to verify the developed code are shown in Table (5.1).

Table 5.1- Parameters used in the first verification case using sand soil

Parameter		Value	Units
θ_r		0.0265	-----
K_{sat}		0.00428	cm/s
ϕ		0.282	-----
van	α	0.044	cm ⁻¹
Genuchten	n	2.2	-----
Top Boundary Condition (Flux)		0.00231	cm/s
Bottom Boundary Condition (Head)		-9.9	cm
Column height		100	cm

Fig. (5.1) shows the results presented by Touma and Vauclin (1986) and Fig. (5.2) shows the corresponding developed model's results. Touma and Vauclin (1986) were simulating two phase flow (i.e. water and air). The soil porosity was 0.312 and they showed that entrapped air can be taken into account by assuming that the soil porosity to be reduced to 0.282. Fig. (5.2) shows the developed model result using porosity of 0.282.

TWO-PHASE INFILTRATION IN A PARTIALLY SATURATED SOIL.

Figure 5.1- Model results of Touma and Vauclin (1986)

Figure 5.2- Developed model results using Touma and Vauclin (1986) parameters

Same soil properties were used by Kennedy (1998) to verify her code. Kennedy (1998) was simulating water saturation only with porosity of 0.312 and she compared her results with Touma and Vauclin (1986) (Fig. (5.1)). Fig. (5.4) shows the model results which match fairly well with the results presented by Kennedy (1998) (Fig. 5.3)). A comparison between Figs. (5.1) and (5.2) and Figs. (5.3) and (5.4) indicates that the flow equation was implemented correctly as the results match fairly well.

5.2.1.2 CASE 2: FLUCTUATING WATER TABLE

Lenhard et al. (1991) conducted an experiment on a 72 cm high sand column. They measured the water pressures using pressures transducers connected to tensiometers and water saturations using a gamma radiation system at various locations in the column (i.e. 70, 60, 50, 40, 30, 20 and 10 cm). The column was under fluctuating water table conditions starting from a fully saturated state with a pressure head of 72 cm at the base of the column and fluctuating according to Fig. (5.5). The upper water boundary condition for the column remained as a no flow boundary however the boundary conditions at the lower end were prescribed pressures that varied according to Fig. (5.5).

The nonhysteretic results reported by Lenhard et al. (1991) that are shown in Fig. (5.6) were compared with the results obtained from the developed code (Fig. (5.7)). Both figures shows similarity which reflects that the flow equations were coded correctly in the developed code.

Figure 5.3- Model results of Kennedy (1998)

Figure 5.4- Developed model results using Kennedy (1998) parameters

Figure 5.5- Case 2, Water pressure fluctuating values for the flow verification.

Table (5.2) shows the soil parameters used to simulate water table fluctuation scenario of Lenhard et al. (1991).

Table 5.2- Soil parameters used for Lenhard et al. (1991)

Parameter		Value	Units
θ_r		0.0612	-----
K_{sat}		0.00331	cm/s
ϕ		0.36	-----
Van	α	0.042	cm ⁻¹
Genuchten	n	5.25	-----
Column height		72	cm

Figure 5.6- Lenhard et al. (1991) model results. Broken curves with alternating short and long segments shows the nonhysteretic solution under concern.

Figure 5.7- Case 2, Developed code results.

5.2.1.3 CASE 3: PEAT SOIL AND FLOW INFILTRATION

Many of the simulations presented later in this thesis simulate the flow, transport and clogging for a peat soil. This is due to the ongoing research efforts at Carleton University to evaluate the clogging of peat filters used to treat septic tank effluent. The flow and transport processes within a peat column are similar to those occurring in other soil types. Adsorption and the impact of a secondary porosity of peat are not included in this research as the focus of this work was to develop conceptual models for an unsaturated clogging. However, for completeness a flow simulation is included here to illustrate the impact of the greater porosity of the peat.

Fig.(5.8) shows the saturation profile for a peat column under similar boundary conditions used for verification case 1. As expected, the saturation profiles advance much slower in peat versus sand because peat has relatively high porosity values. The seepage velocity will be much higher for sand soils due to their lower porosity. The input parameters for the peat simulation are provided in Table (5.3).

Table 5.3- Parameters used in the first verification case using Peat soil

Parameter		Value	Units
θ_r		0.08736	-----
K_{sat}		0.0079	cm/s
ϕ		0.8	-----
van	α	0.18	cm ⁻¹
Genuchten	n	1.3	-----
Top Boundary Condition (Flux)		0.00231	cm/s
Bottom Boundary Condition (Head)		-9.9	cm
Column height		100	cm

The mass balance error for the flow equation was 0.002% over a simulation period of one day, which supports that the flow equation has been coded correctly.

Figure 5.8- Case 3, Flow through peat soil

5.2.2 CONTAMINANT TRANSPORT EQUATION VERIFICATION

As mentioned previously, due to lack of verification simulations for transport in the unsaturated soils, the contaminant transport equation will be verified against a few conceptual cases.

5.2.2.1 CASE 1: VERIFICATION AGAINST ANALYTICAL SOLUTION FOR SAND AND PEAT SOILS

A simulation was conducted on a sand column with soil characteristics shown in Table (5.1). First, the sand column was allowed to reach a steady state flow condition by simulating a flux at the top of the column of 20 cm/day for 6 hours. Then a contaminant

was added to the flux with a concentration of 2000 mg/L for the remainder of the simulation. The simulation was stopped after 5 days and a flow and contaminant mass balance was calculated. The longitudinal dispersivity was assumed to be 1 cm. This scenario can be compared with the analytical solution obtained for a one dimensional advection dispersion equation since the seepage velocities will be constant over the top 70 cm of the column (see Fig. (5.9)). As illustrated in Fig. (5.10), the advective front is at $C/C_0 = 0.5$ which is 1000 mg/L in this case. The contaminant front moves with the flow and the concentration will reach its maximum value along the entire length of the column as the front exits the column as expected. The cumulative flow mass balance error was 0.00% and the cumulative contaminant mass balance error was 0.062% error which gives some indication that the contaminant transport equation was implemented correctly.

It should be noted that the times indicated on Fig.(5.10) are the times from the start of the contaminant injection and not the start of the simulation. As mentioned earlier, the advective front should be at $C/C_0 = 0.5$ and this is clearly defined in Fig. (5.10).

After 0.5 hours from injecting the contaminant, the front should be at 13.91 cm from the top of the column as the Darcy flux is 0.00231 cm/s, the porosity is 0.312, and the saturation is 0.958.

The same scenario was simulated for the peat soil using the same dispersivity values. Fig. (5.11) and (5.12) are the concentration and flow profiles respectively for the peat soil. It should be noted that due to higher porosity value of peat versus sand, the contaminant front will advance slower.

Figure 5.9- Case 1, Flow through sand soil with injection of contaminant after 6 hours

Figure 5.10- Case 1, Contaminant movement in sand soil

Figure 5.11- Case 1, Flow through peat soil with injection of contaminant after 6 hours

Figure 5.12- Case 2, Contaminant movement in peat soil

A cumulative flow mass balance error was 0.00% and cumulative contaminant mass balance error was 0.078% error which gives some indication that the contaminant transport equation was implemented correctly as mentioned previously.

5.2.2.2 CASE 2: FIRST ORDER DECAY RATE

First order decay as a sink term was used to simulate a continuous contaminant source with decay. For the sand column simulation with soil characteristics as shown in Table (5.1), a first order decay rate of 6.93 days^{-1} (half life of 0.1 days) was applied to simulate the decay in the contaminant. Fig. (5.13) shows the concentration profile with distance for various times during the simulation for both the current code and the analytical solution. Again the contaminant injected was initiated after steady state flow was reached as discussed in the previous cases. As expected, there is a reduction in the concentration profile with distance. The cumulative flow mass balance error was 0.00% and the cumulative contaminant mass balance error was 0.01% which supports that the equations were implemented correctly. The simulation was stopped after 10 days as there was no change in the concentration profile since it had reached steady state.

The same scenario was simulated for the peat with half life of 0.1 days. The cumulative flow and contaminant mass balance errors were 0.00%. The concentration profiles with time are shown in Fig. (5.14).

Figure 5.13- Case 2, First order decay rate in a sand soil with half life of 0.1 day

Figure 5.14- Case 2, First order decay rate in a peat soil with half life of 0.1 day

5.3 MODEL RESULTS AND DATA ANALYSIS

5.3.1 SIMULATION OF A PEAT SOIL

The second portion of this chapter deals with the three proposed models for clogging in the unsaturated zone. As discussed previously in chapter 4, the three models link the microbial growth with the relative permeability term. Although the three models

are based on slightly different conceptual theories, the clogging times were found to be relatively close with a difference of a few days for the simulation results shown in this chapter.

A simulation was conducted on a peat column 100 cm high with model input parameters as given in Table (5.4).

Table 5.4- Soil and Monod Kinetics parameters used in the clogging simulation for the peat soil

<i>Soil Properties</i>				<i>Monod Kinetics</i>		
<i>Parameter</i>	<i>Value</i>	<i>Units</i>		<i>Parameter</i>	<i>Value</i>	<i>Units</i>
θ_r	0.08736	-----		Y	0.5	$\frac{mg_{cells}}{mg_{substrate}}$
K_{sat}	0.079	$\frac{cm}{s}$		q_m	0.000005	$\frac{mg_{substrate}}{mg_{cells}} \cdot s$
ϕ	0.8	-----		b	0.000000578	s^{-1}
van Genuchten	α	0.18	cm^{-1}	M_T	1500	$\frac{mg_{cells}}{L}$
	n	1.3 & 3.0	-----	K_s	100	$\frac{mg_{substrate}}{L}$
Column height		100	cm	$\rho_{bacteria}$	1.39	$\frac{gm}{cm^3}$
<i>Stress Period</i>	<i>Starting</i>	<i>Ending</i>	<i>Top B. C.</i>		<i>Bottom B.C.</i>	
1	0.0 s	21600 s	Flux	0.000231 cm/s	Head	-9.9 cm
2	21601 s	Clogging	Flux	0.000231 cm/s	Head	-9.9 cm

The flux was continuously added at the top of the column starting from time zero until the column was clogged. The simulations were automatically stopped when the total saturation reached one which indicates that the microbial growth caused ponding to start at the top of the column. The cumulative flow and contaminant mass balance errors were

found to be 0.058% and 0.59% for Model #1 and 0.034% and 0.19% for Models #2 and 0.035% and 0.22% for Model #3 respectively, using van Genuchten n value of 1.3, which reflects that the developed code is conserving mass reasonably well. It should be noted that the number of divisions used in Model #3 was 20 divisions.

The following figures (Figs (5.15), (5.16), (5.17), (5.18), (5.19) and (5.20)) illustrate the saturation and concentration profiles for Models #1, #2 and #3 respectively using van Genuchten n value of 1.3. It was found that the concentration profiles are fairly similar for the three models. Also, as mentioned before, the clogging times were found to be close for all three model scenarios. It was found that the clogging time for Model #1 was 62.24 days and was 57.62 days for Model #2 and 59.53 days for Model #3.

As mentioned earlier, Model #1 assumed that the smaller pores will fill first with microbes. Since these smaller pores contribute least to the flow, Model #1 should predict the lowest reduction in relative permeability at earlier times and the actual total saturation will not be impacted as much at early times (Fig. (5.15)). For example, after 40 days the actual microbial saturation increased to 20 % with no change in actual total saturation and hence a corresponding decrease in actual water saturation of 20%. No change in the actual total saturation indicates that the 20% actual microbial saturation had little impact on the relative permeability. With time, microbes filled the larger pores and a corresponding impact on the actual total saturation was noticeable. Models #2 and #3 are macroscale and microscale models respectively but with different reduction factors. Since the relative permeability equation is a function of S_{ew} and is further reduced by a reduction factor amount (i.e. $(1 - S_{em})$ factor for Model #2 and the ratio of flow factors for

Figure 5.15- Actual saturation profile for peat soil using Model #1 with van Genuchten n value of 1.3

Figure 5.16- Concentration profile for peat soil using Model #1 with van Genuchten n value of 1.3

Figure 5.17- Actual saturation profile for peat soil using Model #2 with van Genuchten n value of 1.3

Figure 5.18- Concentration profile for peat soil using Model #2 with van Genuchten n value of 1.3

Figure 5.19- Actual saturation profile for peat soil using Model #3 with van Genuchten n value of 1.3

Figure 5.20- Concentration profile for peat soil using Model #3 with van Genuchten n value of 1.3

Model #3), a significant impact will occur on the total saturation values at earlier times. In comparison with the results of Model #1, after 40 days the microbial saturation predicted using Models #2 and #3 also increased to 20%. However, the total saturation also increased by approximately 10% to account for the reduction in relative permeability caused by the microbial growth.

Clogging was faster for Model #2 versus Model #3 as the $(1 - S_{em})$ factor generated a greater reduction in the relative permeability values versus the flow factor in Model #3. This can be seen in Fig. (5.21) as the minimum value of the flow factor was approximately 0.95 however it was approximately 0.47 using Model #2. By using a higher value for the van Genuchten n parameter, the flow factor is noticeably reduced which supports what was previously discussed in Chapter 4. The same simulations were conducted using Models #2 and #3 using a van Genuchten n value of 3.0. Fig. (5.22) shows a comparison between the $(1 - S_{em})$ factor and the flow factor for the higher n value. The minimum value of the flow factor was approximately 0.17 for Model #3 and 0.13 for Model #2. The clogging times for Models #2 and #3 were found to be very close.

As was noted earlier, clogging occurred when the actual total saturation reached 100% in the top grid block. Since the impact on the actual total saturation for Model #1 was not as large as for Models #2 and #3, it took longer for the simulation using Model #1 to reach a clogging state. In addition, at clogging, the actual microbial saturation simulated using Model #1 (approximately 90%) was much greater than the actual microbial saturation simulated using Models #2 and #3 (approximately 50%).

Figure 5.21- Comparison between the $(1 - S_{em})$ factor and the flow factor using van Genuchten n value of 1.3

Figure 5.22- Comparison between the $(1 - S_{em})$ factor and the flow factor using van Genuchten n value of 3.0

Clogging will be faster in Models #2 and #3 versus #1. As stated earlier, for Model #1 the effect of microbial growth will not be significant at earlier times and only when the actual microbial saturation is significant, will the relative permeability be impacted. Fig. (5.23) supports this conceptual idea as a significant reduction in the

relative permeability started at about 37 days when the effective microbial saturation was approximately 0.18 (i.e. 0.16 actual microbial saturation). The actual total saturation increased at later times (i.e. 60 days) as shown in Fig. (5.15) and Fig. (5.23) and it reached 100% in the last 2 days of the simulation. It should be noted that there is a slight increase in S_{et} at earlier times. This slight increase is not obvious in Fig. (5.23) due to the scale of this figure.

Figure 5.23- Relative Permeability, effective total, water and microbial saturations versus time at the top 0.5 cm of the peat column using Model #1 with van Genuchten n value of 1.3

In Models #2 and #3, the impact on the relative permeability was different. A significant impact occurred at earlier times (Fig. (5.24) for Model #2 and Fig. (5.25) for Model #3). The relative permeability started to decrease when the effective microbial saturation was approximately 0.006 (i.e. 0.005 actual microbial saturation) at 12 days for Model #2 and at approximately the same saturation for Model #3. The effective total saturation increased to compensate for the reduced permeability and it reached 100%

while the effective microbial saturation reached approximately 53.6% for Model #2 and approximately 57.3% for Model #3.

Figure 5.24- Relative Permeability, effective total, water and microbial saturations versus time at the top 0.5 cm of the peat column using Models #2 with van Genuchten n value of 1.3

Figure 5.25- Relative Permeability, effective total, water and microbial saturations versus time at the top 0.5 cm of the peat column using Models #3 with van Genuchten n value of 1.3

It was also noted in the literature that clogging occurred in the top 1 to 2 cm of a soil column when continuously loaded with an organic source. The simulation results presented here indicate the same trend. For Models #1, #2 and #3 more than 95% of the microbial growth occurred within the top 1.5 cm of the soil column.

5.3.2 SIMULATION ON A SAND SOIL

Another simulation was conducted for a 100 cm sand column using Models #1 and #2. The saturation and the concentration profiles for Models #1 and #2 are given in Figs. (5.26), (5.27), (5.28) and (5.29) respectively.

For a porosity of 0.3 for the sand soil, clogging will occur faster versus the peat soil as microbes only have to occupy this smaller porosity versus the greater one in the peat. Using Model #1, clogging occurs after 43.98 days with a cumulative flow mass balance error of 0.053% and a cumulative contaminant mass balance error of 1.03% while clogging occurs after 43.09 days using Model #2 with a flow mass balance error of 0.045% and a contaminant mass balance error of 0.38%.

It is also worth noting the distribution of the microbial growth in the sand versus peat simulations. As discussed earlier, Figs. (5.15), (5.17) and (5.19) indicate that greater than 95% of the microbial mass is located in the top 1.5 cm of the peat column. In comparison, Figs. (5.26) and (5.28) indicate that the microbial mass is distributed over a greater depth of 4-5 cm due to the lower porosity.

As the porosity decreases, the seepage velocity increases which allows the substrate to penetrate faster and further into the column. As the microbial mass increases,

Figure 5.26- Actual saturation profile for sand soil using Model #1

Figure 5.27- Concentration profile for sand soil using Model #1

Figure 5.28- Actual saturation profile for sand soil using Model #2

Figure 5.29- Concentration profile for sand soil using Model #2

the degradation rate also increases however it never reaches the degradation rate in the peat column since the sand column clogs more rapidly. The slower degradation rate at the time of clogging and the higher seepage velocity allow the contaminant to advance further into the column to establish the larger zone of microbial growth.

Also, by comparing Figs. (5.30) and (5.31), the trends in the relative permeability for the simulation with sand are similar to the simulation results for peat.

The reduction in the relative permeability started earlier in Model #2 (Fig. (5.31)) versus Model #1 (Fig. (5.30)) as any microbial growth will significantly impact the total saturation for Model #2 as discussed earlier for the peat soil scenario.

Figure 5.30- Relative Permeability, effective total, water and microbial saturations versus time at the top 0.5 cm of the sand column using Model #1

Figure 5.31- Relative Permeability, effective total, water and microbial saturations versus time at the top 0.5 cm of the sand column using Model #2

5.3.3 PULSE SIMULATION

As discussed previously, one of the most important applications for clogging is septic systems. The peat filters designed to treat larger volumes of septic tank effluent at schools (Kennedy and Van Geel, 2001), for example, or to treat smaller volumes at a home (Ecoflo® Biofilters, Premier Tech. Environment), generally pulse the system to decrease the chances of a thin biomat at the surface.

As seen in the previous simulations, a low continuous flux results in a very shallow biomat which clogs a column very quickly. If the same hydraulic and organic loading is applied in 2-3 pulses rather than continuously throughout a period of a day, the organic source can advance further into the column prior to degrading and hence the microbial mass needed to degrade the organic load will distribute itself over a greater depth.

Figure 5.32- Saturation profile for pulsing simulation on a peat column

To illustrate the impacts of microbial growth, several simulations were completed and the impact of microbial growth on the moisture content profile can be seen when the moisture content profile was plotted at various times.

Table (5.6) shows the Monod kinetic parameters used in the different simulations in which a peat column was pulsed for 6 months. It was found that with the pulsing scenario, it was difficult to reach a clogging scenario within a six month period for a peat column loaded with the same hydraulic and organic loading as the continuous conditions presented earlier. Increasing, substrate concentrations from 2000 mg/L to 20,000 mg/L for a 6-month period using the same Monod kinetics did not result in clogging. The Monod kinetics had a significant impact in the microbial saturation and were varied as

shown in Table (5.6) to illustrate their impact on microbial saturation. However, a clogging scenario was not generated for a 6-month simulation.

Figs. (5.33), (5.34), (5.35) and (5.36) show the simulation results for the four scenarios of pulsing a peat column using conceptual Model #1. In the first pulsing scenario, there is a very little effect on the saturation profile due to microbial growth. The largest microbial saturation value can be found at the top of the column at the end of 6 months and it is about 0.012 (Fig. (5.33)).

When the initial microbial concentration was increased 10 times and the substrate concentration was increased 2.5 times versus the first case, the microbial saturation profile did not show a significant increase (Fig. (5.34)). A maximum microbial saturation of 0.029 was simulated at the top of the column after 6 months of pulse loading.

When the substrate concentration was increased to 10,000 mg/L, the microbial saturation increased to 0.061 which can be seen in Fig. (5.35).

A noticeable increase in the microbial saturation and a corresponding reduction in the water saturation were simulated based on the set of parameters used in the forth pulsing scenario (Fig. (5.36)). As can be noticed, the initial concentration of microbes was increased and the maximum rate of substrate utilization as well. The effect of the initial microbial concentration in the column had less affect than the kinetics parameters on the microbial growth over time.

Table 5.6- Monod Kinetics parameters used for several attempts in pulsing a peat column for 6 month

<i>Simulation</i>	<i>Criteria</i>	<i>Top B. C.</i>		<i>Bottom B.C.</i>	
<i>1</i>	Loading for 15 min every 12 hours for 6 month	Flux	0.011111 cm/s	Head	-9.9 cm
<i>Monod Kinetics Parameters with substrate concentration of 2000 mg/L</i>					
<i>Parameter</i>	Y	q_m	b	M_T	K_s
<i>Value</i>	0.5	0.000005	0.000000578	1500	100
<i>Units</i>	$\frac{mg_{cells}}{mg_{substrate}}$	$\frac{mg_{substrate}}{mg_{cells}} \cdot s$	s^{-1}	$\frac{mg_{cells}}{L}$	$\frac{mg_{substrate}}{L}$
<i>Simulation</i>	<i>Criteria</i>	<i>Top B. C.</i>		<i>Bottom B.C.</i>	
<i>2</i>	Loading for 15 min every 12 hours for 6 month	Flux	0.011111 cm/s	Head	-9.9 cm
<i>Monod Kinetics Parameters with substrate concentration of 5000 mg/L</i>					
<i>Parameter</i>	Y	q_m	b	M_T	K_s
<i>Value</i>	0.5	0.000005	0.000000578	15000	100
<i>Units</i>	$\frac{mg_{cells}}{mg_{substrate}}$	$\frac{mg_{substrate}}{mg_{cells}} \cdot s$	s^{-1}	$\frac{mg_{cells}}{L}$	$\frac{mg_{substrate}}{L}$
<i>Simulation</i>	<i>Criteria</i>	<i>Top B. C.</i>		<i>Bottom B.C.</i>	
<i>3</i>	Loading for 15 min every 12 hours for 6 month	Flux	0.011111 cm/s	Head	-9.9 cm
<i>Monod Kinetics Parameters with substrate concentration of 10,000 mg/L</i>					
<i>Parameter</i>	Y	q_m	b	M_T	K_s
<i>Value</i>	0.5	0.000005	0.000000578	1500	100
<i>Units</i>	$\frac{mg_{cells}}{mg_{substrate}}$	$\frac{mg_{substrate}}{mg_{cells}} \cdot s$	s^{-1}	$\frac{mg_{cells}}{L}$	$\frac{mg_{substrate}}{L}$

Table 5.6 Cont'd- Monod Kinetics parameters used for several attempts in pulsing a peat column for 6 month

<i>Simulation</i>	<i>Criteria</i>	<i>Top B. C.</i>		<i>Bottom B.C.</i>	
4	Loading for 15 min every 12 hours for 6 month	Flux	0.011111 cm/s	Head	-9.9 cm
<i>Monod Kinetics Parameters with substrate concentration of 20,000 mg/L</i>					
<i>Parameter</i>	Y	q_m	b	M_T	K_s
<i>Value</i>	0.5	0.00005	0.000000578	15000	100
<i>Units</i>	$\frac{mg_{cells}}{mg_{substrate}}$	$\frac{mg_{substrate}}{mg_{cells}} \cdot s$	s^{-1}	$\frac{mg_{cells}}{L}$	$\frac{mg_{substrate}}{L}$

Figure 5.33- First pulsing scenario of a peat column; influent concentration of 2000 mg/L, initial microbial concentration of 1500 mg/L

Figure 5.34- Second pulsing scenario of a peat column; influent concentration of 5000 mg/L, initial microbial concentration of 15000 mg/L

Figure 5.35- Third pulsing scenario of a peat column; influent concentration of 10000 mg/L, initial microbial concentration of 1500 mg/L

Figure 5.36- Forth pulsing scenario of a peat column; influent concentration of 20000 mg/L, initial microbial concentration of 15000 mg/L

6 CONCLUSION

Many conceptual models are presented in the literature for clogging in the saturated zone but similar models for the unsaturated zone are limited. This research proposed three new conceptual models that relate the microbial growth to the relative permeability of the soil. The three models used the approach proposed by Burdine (1953) and Mualem (1976) as a base relationship between the relative permeability and the saturation of the soil.

Model #1 was based on a modification to the integration proposed by Burdine and Mualem to account for the presence of microbial mass. In this model, a microbial mass was assumed to occupy a portion of the pore space which reduces the relative permeability for a given water saturation. As the microbial mass fills the smaller water-filled pores, the flow is displaced to the larger pores to compensate for the reduced permeability. This process can continue until all the pores are filled with bacteria cells and the soil becomes fully clogged. Since it was assumed that the smaller pores are filled first and these pores contribute the least to the flow, there is no significant impact on the relative permeability term until a sufficient microbial mass is generated to significantly affect the flow path.

Model #2 used the same equation presented by Burdine and Mualem, and microbial growth was taken into account by reducing the relative permeability by a factor of $(1 - S_{em})$. Any slight increase in the microbial mass will result in a reduction in the relative permeability and a corresponding increase in the actual total saturation to conduct the flow.

Model #3 was based on a biofilm approach where a new flow factor term was introduced to account for the reduced flow through the capillary tubes when a biofilm lined the walls of the capillary tubes. In this model, the microbial mass is assumed to distribute itself uniformly within the capillary tubes of the porous medium regardless of the water saturation since all the pores contain at least an irreducible water saturation and can accommodate microbial growth. This model used the same equation presented by Burdine and Mualem multiplied by a flow reduction factor based on laminar flow (Hagen Poiseuille) in the capillary tubes with and without a biofilm. An increase in microbial mass decreases the relative permeability which in turn results in an increase in the total saturation to conduct the applied flux.

A one dimensional, unsaturated flow and transport code was developed as a part of this research to study the effect of the different conceptual models on the clogging of unsaturated soil. Two different soil types, sand and peat, were simulated to illustrate the functionality of the code. Sand soil was chosen as it is often used as a filter medium and peat was selected because it has become a common filter medium used with septic systems. In addition, these two soils have different porosities which helps to illustrate the impact of porosity on the clogging processes within a filter.

Continuous and pulsed load scenarios were simulated to illustrate the effect of continuous and pulsed loading on clogging. It was clearly demonstrated that for the same daily hydraulic and organic loading, continuous loading resulted in clogging much sooner than pulsed loading due to the formation of a thin biomat at the influent surface. For continuous loading, sand soils will clog faster than the peat columns due to their lower porosity.

In addition, for the same soil type, the clogging time to reach clogging was similar (i.e. within a few days) for each of the proposed models. The impact of the microbial growth on the actual total saturation was larger in Models #2 and #3 versus Model #1, as expected, and this resulted in slightly faster clogging times for Models #2 and #3. Also, the effect of the van Genuchten n value (i.e. a well graded soil having a greater n value versus a well sorted soil having a lower n value) was discussed as a well sorted soil results in a lower flow factor and a greater reduction of the relative permeability term for a give microbial saturation.

Further research should be conducted to verify these conceptual models. More experimental work should be conducted on laboratory soil columns under known organic and hydraulic loading rates. Peat and sand soils can be used in the columns and can be tested at different densities and different organic substrate loading to simulate biological clogging in peat biofilters. Available devices (i.e. Time Domain Reflectometer (TDR)) will be used to measure the saturation profile with depth in order to record the increase in total saturation due to increase in the microbial saturation. The measured saturation profiles could be compared to the simulated profiles to verify the proposed conceptual models. Soil samples at varying degrees of clogging should be investigated at the microscopic level using advanced techniques from biology or earth sciences. Also, more conceptual models should be developed to increase our understanding of clogging in unsaturated soils.

From a numerical and technical point of view, different microbial growth kinetics should be investigated and compared with the results proposed in this research using

Monod kinetics. Also, different numerical techniques should be investigated as the finite difference technique used in this research is not the only technique to use.

Hysteresis is an important phenomenon that should be considered as well in the future work as continuous cycles of wetting and draining may affect the clogging process in unsaturated soils.

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APPENDIX A – MATHEMATICAL DERIVATION

A.1 EQUATIONS BASED ON BURDINE'S MODEL

In 1953, Burdine developed an integral equation that expresses the relation between the relative permeability and the saturation of the soil,

$$k_r(S_e) = S_e^2 \frac{\int_{S_e=0}^{S_e} \frac{dS_e}{\psi^2}}{\int_{S_e=0}^1 \frac{dS_e}{\psi^2}} \quad (\text{A.1})$$

where $k_r(S_e)$ is the relative permeability, S_e is the effective saturation and ψ in the capillary pressure. The capillary pressure can be related to the saturation using a relationship proposed by van Genuchten (1980),

$$S_e = \frac{1}{\left(1 + (\alpha\psi)^n\right)^m} \quad (\text{A.2})$$

where n , m and α are fitting parameters for this relationship. Also,

$$m = 1 - \frac{2}{n} \quad (\text{A.3})$$

is assumed as a relation between m and n .

Using equation (A.2), if we assume $\psi = \alpha\psi$, a relation between the capillary pressure and effective saturation can be determined in the form of $\psi = \psi(S_e)$ as follows,

$$S_e^{1/m} = \frac{1}{\left(1 + (\psi)^n\right)},$$

$$1 + (\psi)^n = \frac{1}{S_e^{1/m}},$$

$$(\psi)^n = \frac{1}{S_e^{1/m}} - 1,$$

$$(\psi)^n = \frac{1 - S_e^{1/m}}{S_e^{1/m}},$$

$$(\psi) = \left(\frac{1 - S_e^{1/m}}{S_e^{1/m}} \right)^{1/n},$$

$$\therefore (\psi)^2 = \left(\frac{1 - S_e^{1/m}}{S_e^{1/m}} \right)^{2/n} \quad (\text{A.4})$$

So, equation (A.1) can be rewritten in the form,

$$k_r(S_e) = S_e^2 \left(\frac{f(S_e)}{f(l)} \right) \quad (\text{A.5})$$

as

$$f(S_e) = \int_0^{S_e} \frac{dS_e}{(\psi)^2},$$

$$f(S_e) = \int_0^{S_e} \left(\frac{S_e^{1/m}}{1 - S_e^{1/m}} \right)^{2/n} dS_e$$

$$f(S_e) = \int_0^{S_e} \left((S_e)^{1/m} \right)^{2/n} \cdot \left(1 - (S_e)^{1/m} \right)^{-2/n} dS_e \quad (\text{A.6})$$

substituting with $S_e = y^m$ into equation(A.6) gives,

$$f(S_e) = \int_0^{S_e^{1/m}} \left((y^m)^{1/m} \right)^{2/n} \cdot \left(1 - (y^m)^{1/m} \right)^{-2/n} m y^{m-1} dy$$

$$f(S_e) = m \int_0^{S_e^{1/m}} y^{m-1+\frac{2}{n}} (1-y)^{-2/n} dy \quad (\text{A.7})$$

Equation (A.7) is difficult to integrate except for certain restrictions (van

Genuchten 1980). Using $m=1-\frac{2}{n}$ as a condition for the integration as,

$$m-1 = \frac{-2}{n}$$

$$n = \frac{2}{1-m} \quad (\text{A.8})$$

and substitute with equation (A.8) into equation (A.7) leads to,

$$f(S_e) = m \int_0^{S_e^{1/m}} y^{m-1+1-m} (1-y)^{-(1-m)} dy$$

$$f(S_e) = m \int_0^{S_e^{1/m}} (1-y)^{(m-1)} dy$$

$$f(S_e) = m \left(\frac{-1}{m} (1-y)^{(m-1)} \right) \Bigg|_0^{S_e^{1/m}}$$

$$f(S_e) = -(1-S_e^{1/m})^m - (-(1-0)^m)$$

$$f(S_e) = -(1-S_e^{1/m})^m + 1$$

$$\therefore f(S_e) = 1 - (1-S_e^{1/m})^m \quad (\text{A.9})$$

Then from equation (A.9) and because $f(l) = 1$, equation (A.5) becomes,

$$k_r(S_e) = S_e^2 \left(1 - (1-S_e^{1/m})^m \right) \quad \begin{cases} m = 1 - \frac{2}{n} \\ 0 < m < 1, n > 2 \end{cases} \quad (\text{A.10})$$

A.2 EQUATIONS BASED ON MUALEM'S MODEL

In 1978, Mualem developed an integral equation, which was slightly different than Burdine's (1953), that expresses the relation between the relative permeability and the saturation of the soil,

$$k_r(S_e) = S_e^{1/2} \left(\frac{\int_{S_e=0}^{S_e} \frac{dS_e}{\psi}}{\int_{S_e=0}^1 \frac{dS_e}{\psi}} \right)^2 \quad (\text{A.11})$$

where $k_r(S_e)$ is the relative permeability, S_e is the effective saturation and ψ in the capillary pressure. The capillary pressure can be related to the saturation using the van Genuchten relationship (van Genuchten, 1980),

$$S_e = \frac{1}{(1 + (\alpha\psi)^n)^m} \quad (\text{A.12})$$

where n , m and α are fitting parameters for this relationship. Also,

$$m = 1 - \frac{1}{n} \quad (\text{A.13})$$

is assumed as a relation between m and n .

As before in Burdine equations (A.12), if we assume $\psi = \alpha\psi$, can be used to obtain a relation between the capillary pressure and effective saturation in the form of $\psi = \psi(S_e)$ as,

$$(\psi) = \left(\frac{1 - S_e^{1/m}}{S_e^{1/m}} \right)^{1/n} \quad (\text{A.14})$$

So, equation (11) can be rewritten in the form,

$$k_r(S_e) = S_e^{1/2} \left(\frac{f(S_e)}{f(l)} \right)^2 \quad (\text{A.15})$$

as

$$f(S_e) = \int_0^{S_e} \frac{dS_e}{\psi},$$

$$f(S_e) = \int_0^{S_e} \left(\frac{S_e^{1/m}}{1 - S_e^{1/m}} \right)^{1/n} dS_e$$

$$f(S_e) = \int_0^{S_e} \left((S_e)^{1/m} \right)^{1/n} \cdot \left(1 - (S_e)^{1/m} \right)^{-1/n} dS_e \quad (\text{A.16})$$

substituting with $S_e = y^m$ into equation (A.16) gives,

$$\begin{aligned} f(S_e) &= \int_0^{S_e^{1/m}} \left((y^m)^{1/m} \right)^{1/n} \cdot \left(1 - (y^m)^{1/m} \right)^{-1/n} m y^{m-1} dy \\ f(S_e) &= m \int_0^{S_e^{1/m}} y^{m-1+\frac{1}{n}} (1-y)^{-1/n} dy \end{aligned} \quad (\text{A.17})$$

Equation (A.17) is difficult to integrate except for certain restrictions (van Genuchten 1980). Using $m = 1 - \frac{1}{n}$ as a condition for the integration as,

$$\begin{aligned} m-1 &= \frac{-1}{n} \\ n &= \frac{1}{1-m} \end{aligned} \quad (\text{A.18})$$

and substitute with equation (A.18) into equation (A.17) leads to,

$$f(S_e) = m \int_0^{S_e^{1/m}} y^{m-1+1-m} (1-y)^{-(1-m)} dy$$

$$f(S_e) = m \int_0^{S_e^{1/m}} (1-y)^{(m-1)} dy$$

$$f(S_e) = m \left(\frac{-1}{m} (1-y)^{(m-1)} \right) \Bigg|_0^{S_e^{1/m}}$$

$$f(S_e) = -(1-S_e^{1/m})^m - (-(1-0)^m)$$

$$f(S_e) = -(1-S_e^{1/m})^m + 1$$

$$\therefore f(S_e) = 1 - (1-S_e^{1/m})^m \quad (\text{A.19})$$

Then from equation (A.19) and because $f(l) = 1$, equation (A.15) becomes,

$$k_r(S_e) = S_e^{1/2} \left(1 - (1 - S_e^{1/m})^m\right)^2 \quad \begin{cases} m = 1 - \frac{1}{n} \\ 0 < m < 1 \end{cases} \quad (\text{A.20})$$

A.3 PROPOSED RELATIVE PERMEABILITY - SATURATION RELATIONSHIP ACCORDING TO BURDINE'S MODEL

The integral equation according to Burdine's model will be in the form,

$$k_r(S_{ew}) = S_{et}^2 \frac{\int_0^{S_{et}} \frac{dS_e}{\psi^2} - \int_0^{S_{em}} \frac{dS_e}{\psi^2}}{\int_{S_e=0}^1 \frac{dS_e}{\psi^2}} \quad (\text{A.21})$$

and equation (A.21) can be rewritten in the form,

$$k_r(S_{ew}) = S_{et}^2 \left(\frac{f(S_{et}) - f(S_{em})}{f(l)} \right) \quad (\text{A.22})$$

Using Equation (A.4) leads to,

$$f(S_{et}) = \int_0^{S_{et}} \left(\frac{dS_e}{\psi^2} \right) = \int_0^{S_{et}} \left(\frac{S_{et}^{1/m}}{1 - S_{et}^{1/m}} \right)^{2/n} dS_e \quad (\text{A.23})$$

and,

$$f(S_{em}) = \int_0^{S_{em}} \left(\frac{dS_e}{\psi^2} \right) = \int_0^{S_{em}} \left(\frac{S_{em}^{1/m}}{1 - S_{em}^{1/m}} \right)^{2/n} dS_e \quad (\text{A.24})$$

Substituting $S_{et} = S_{em} = y^m$ in both equations (A.23) and (A.24) leads to,

$$f(S_{ew}) = m \int_0^{S_{et}^{1/m}} y^{m-1+\frac{2}{n}} (1-y)^{-2/n} dy \quad (\text{A.25})$$

and,

$$f(S_{em}) = m \int_0^{S_{em}^{1/m}} y^{m-1+\frac{2}{n}} (1-y)^{-2/n} dy \quad (\text{A.26})$$

If we use $m = 1 - \frac{2}{n}$ then,

$$f(S_{et}) = 1 - (1 - S_{et}^{1/m})^m \quad (\text{A.27})$$

and,

$$f(S_{em}) = 1 - (1 - S_{em}^{1/m})^m \quad (\text{A.28})$$

and because $f(l) = 1$, equation (22) becomes,

$$k_r(S_{ew}) = S_{et}^2 \left(\left(1 - (1 - S_{et}^{1/m})^m \right) - \left(1 - (1 - S_{em}^{1/m})^m \right) \right) \quad (\text{A.29})$$

Rearranging equation (29) leads to,

$$k_r(S_{ew}) = S_{et}^2 \left((1 - S_{em}^{1/m})^m - (1 - S_{et}^{1/m})^m \right) \quad (\text{A.30})$$

where S_{ew} is the effective water saturation, S_{em} is the effective microbial saturation and S_{et} is the effective total saturation.

Equation (A.30) is the final form of the relative permeability saturation relationship for the proposed biological clogging model according to Burdine's model.

A.4 PROPOSED RELATIVE PERMEABILITY - SATURATION RELATIONSHIP ACCORDING TO MUALEM'S MODEL

The integral equation according to Mualem's model will be in the form,

$$k_r(S_{ew}) = S_{et}^{1/2} \left(\frac{\int_0^{S_{et}} \frac{dS_e}{\psi} - \int_0^{S_{em}} \frac{dS_e}{\psi}}{\int_{S_e=0}^1 \frac{dS_e}{\psi}} \right)^2 \quad (\text{A.31})$$

and equation (A.31) can be rewritten in the form,

$$k_r(S_{ew}) = S_{et}^{1/2} \left(\frac{f(S_{et}) - f(S_{em})}{f(1)} \right)^2 \quad (\text{A.32})$$

Using Equation (A.14) leads to,

$$f(S_{et}) = \int_0^{S_{et}} \left(\frac{dS_e}{\psi} \right) = \int_0^{S_{et}} \left(\frac{S_{et}^{1/m}}{1 - S_{et}^{1/m}} \right)^{1/n} dS_e \quad (\text{A.33})$$

and,

$$f(S_{em}) = \int_0^{S_{em}} \left(\frac{dS_e}{\psi} \right) = \int_0^{S_{em}} \left(\frac{S_{em}^{1/m}}{1 - S_{em}^{1/m}} \right)^{1/n} dS_e \quad (\text{A.34})$$

Substituting $S_{et} = S_{em} = y^m$ in both equations (A.33) and (A.34) leads to,

$$f(S_{et}) = m \int_0^{S_{et}^{1/m}} y^{m-1+\frac{1}{n}} (1-y)^{-1/n} dy \quad (\text{A.35})$$

and,

$$f(S_{em}) = m \int_0^{S_{em}^{1/m}} y^{m-1+\frac{1}{n}} (1-y)^{-1/n} dy \quad (\text{A.36})$$

If we use $m = 1 - \frac{1}{n}$ then,

$$f(S_{et}) = 1 - (1 - S_{et}^{1/m})^m \quad (\text{A.37})$$

and,

$$f(S_{em}) = 1 - (1 - S_{em}^{1/m})^m \quad (\text{A.38})$$

and because $f(l) = 1$, equation (A.32) becomes,

$$k_r(S_{ew}) = S_{et}^{1/2} \left(\left(1 - (1 - S_{et}^{1/m})^m \right) - \left(1 - (1 - S_{em}^{1/m})^m \right) \right)^2 \quad (\text{A.39})$$

Rearranging equation (A.39) leads to,

$$k_r(S_{ew}) = S_{et}^{1/2} \left((1 - S_{em}^{1/m})^m - (1 - S_{et}^{1/m})^m \right)^2 \quad (\text{A.40})$$

Equation (A.40) is the final form of the relative permeability saturation relationship for the proposed biological clogging model according to Mualem's model.

A.5 TRANSFORM VAN GENUCHTEN RELATIONSHIP TO SOLVE FOR THE CAPILLARY PRESSURES

The original equation of van-Genuchten relationship is as follows,

$$S_e = \left(1 + (\alpha\psi)^n \right)^{-m} \quad (\text{A.41})$$

then,

$$S_e^{-\frac{1}{m}} = \left(1 + (\alpha\psi)^n \right) \quad (\text{A.42})$$

By moving the capillary pressure term to the left hand side of the equation and the remaining terms to the right hand side we obtain,

$$(\alpha\psi)^n = S_e^{-\frac{1}{m}} - 1 \quad (\text{A.43})$$

then solving for the capillary pressure will gives,

$$\psi = \frac{\left(S_e^{\frac{-1}{m}} - 1\right)^{\frac{1}{n}}}{\alpha} \quad (\text{A.44})$$

Using equation (A.44), capillary pressure values can be obtained for any corresponding saturation values.

A.6 NEWTON-RAPHSON TECHNIQUE

Newton-Raphson technique is used to solve nonlinear equations like the flow equation described earlier in chapter 3 (Dennis and Schnabel 1983).

For any given function, $f(x)$, if the first guess or the initial estimate of the solution at a certain time is given by x_i , a better estimate, x_n , can be obtained by drawing a tangent to the function $f(x)$ at this initial guess as,

$$x_n = x_i - \Delta x \quad (\text{A.45})$$

and

$$f'(x_i) = \frac{\Delta y}{\Delta x} = \frac{f(x_i)}{\Delta x} \quad (\text{A.46})$$

then

$$f'(x_i) \Delta x = \Delta y = f(x_i) \quad (\text{A.47})$$

or

$$x_n = x_i - \frac{f(x_i)}{f'(x_i)} \quad (\text{A.48})$$

Fig. (A.1) shows graphically the parameters used in the previous explanation of Newton-Raphson technique.

In the proposed code, Newton-Raphson technique solves for the total head values seeking a difference between two consequent estimates of heads to be less than a prescribed δ value.

Basically, the solution for the flow equation is achieved when,

$$f(h)=0 \quad (\text{A.49})$$

and δ is obtained using

$$\delta = \frac{-f(h)}{f'(h)} \quad (\text{A.50})$$

The values of the total head (h^t) will be known and we are seeking $h^{t+\Delta t}$.

The solution will be based on increasing the solution by a certain value Δh to obtain $h_1^{(t+\Delta t)}$ and this value will be the first guess such that,

$$h_1^{(t+\Delta t)} = h^t + \Delta h \quad (\text{A.51})$$

Solving for δ gives

$$\delta_1 = \frac{-f(h_1^{(t+\Delta t)})}{f'(h_1^{(t+\Delta t)})} \quad (\text{A.52})$$

and if δ_1 is less than δ , the solution at this time step will be $h_1^{(t+\Delta t)}$ otherwise, a $h_1^{(t+\Delta t)}$ has to be adjusted again hence,

$$h_2^{(t+\Delta t)} = h_1^{(t+\Delta t)} + \Delta h \quad (\text{A.53})$$

and resolving for δ gives

$$\delta_2 = \frac{-f(h_2^{(t+\Delta t)})}{f'(h_2^{(t+\Delta t)})} \quad (\text{A.54})$$

Check again whether δ_2 is less than δ or not and so on.

Figure A.1- One iteration using Newton-Raphson technique

It should be noted that the derivative values at any time step can be calculated as

$$f'(h_i^{(t+\Delta t)}) = \frac{f(h_i^{(t+\Delta t)} + \Delta h) - f(h_i^{(t+\Delta t)})}{\Delta h} \quad (\text{A.55})$$

A.7 THOMAS-ALGORITHM AND FUNCTION DERIVATIVE

As shown in the Newton-Raphson technique, the generated derivative function values are in a form of a tri-diagonal matrix. To solve for δ values, the Thomas algorithm should be used as,

$$[\text{Derivatives}] \{ \delta \} = \{ \text{function} \} \quad (\text{A.56})$$

where the derivative matrix is a tri-diagonal matrix, the vector $\{ \delta \}$ is the unknowns and the vector $\{ \text{function} \}$ is the assumed values of the functions.

The mathematical explanation of Thomas algorithm follows:

Any tri-diagonal matrix $[A]$,

$$A = \begin{bmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \\ & & a_n & b_n \end{bmatrix} \quad (\text{A.57})$$

can be divided into two multiplied matrices in the form,

$$[L] [U] = [A] \quad (\text{A.58})$$

as

$$\begin{bmatrix} 1 & & & \\ d_2 & 1 & & \\ & \ddots & \ddots & \\ & & d_n & 1 \end{bmatrix} \begin{bmatrix} e_1 & f_1 & & \\ e_2 & f_2 & & \\ & \ddots & \ddots & \\ & & e_n & f_n \end{bmatrix} = \begin{bmatrix} e_1 & f_1 & & \\ d_2 e_1 & (d_2 f_1 + e_2) & f_2 & \\ & d_2 e_2 & (d_3 f_2 + e_3) & f_3 \\ & & 0 & \ddots \end{bmatrix} \quad (\text{A.59})$$

by equating matrices in Eq. (A.57) and Eq. (A.59) gives,

$$f_i = c_i \quad (\text{A.60})$$

$$e_i = b_i \quad (\text{A.61})$$

$$d_i = \frac{a_i}{e_i - 1} \quad i = 2, 3, \dots, n \quad (\text{A.62})$$

$$e_i = b_i - d_i c_{i-1} \quad i = 2, 3, \dots, n \quad (\text{A.63})$$

then solve as

$$[A] \{X\} = \{B\} \quad (\text{A.64})$$

and conducting forward substitution yields,

$$\begin{bmatrix} 1 & & & \\ d_2 & 1 & & \\ & & \ddots & \\ & & & d_n & 1 \end{bmatrix} \begin{Bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{Bmatrix} = \begin{Bmatrix} k_1 \\ k_2 \\ \vdots \\ k_n \end{Bmatrix} \quad (\text{A.65})$$

where

$$g_1 = k_1 \quad (\text{A.66})$$

$$g_i = k_i - d_i g_{i-1} \quad i = 2, 3, \dots, n \quad (\text{A.67})$$

then conducting backward substitution yields,

$$\begin{bmatrix} e_1 & c_1 & & \\ & e_2 & c_2 & \\ & & \ddots & \\ & & & e_{n-1} & c_{n-1} \\ & & & & e_n \end{bmatrix} \begin{Bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{Bmatrix} = \begin{Bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{Bmatrix} \quad (\text{A.68})$$

where

$$X_n = \frac{g_n}{e_n} \quad (\text{A.69})$$

$$X_i = \frac{g_i - c_i X_{i+1}}{e_i} \quad i = n-1, \dots, 1 \quad (\text{A.70})$$

and the vector $\{X\}$ is the required vector (i.e. vector $\{\delta\}$).

A.8 FINITE DIFFERENCE DERIVATION “CENTRAL WEIGHTING”

As mentioned in subsection 3.2.3.5, the finite difference technique is similar to control volume approach. In the control volume approach, the conservation of mass equation is applied to a specified control volume. Fig. (A.2) shows the grid block discretization.

Figure A.2- Central and upstream weighting discretization.

The one dimensional advection dispersion equation in the unsaturated soil zone is as follows,

$$\frac{\partial C}{\partial t} = \frac{\partial^2 (D.C)}{\partial z^2} - \frac{\partial \left(\frac{q}{\phi S_w} . C \right)}{\partial z} \quad (\text{A.71})$$

where C is the concentration of the substrate, D is the dispersion coefficient, q is the Darcy flux, ϕ is the porosity, S_w is the actual water saturation and z is the distance measured positive upward.

Conducting the mass balance at grid block i shown in Fig. (A.2) yields,

$$\left(\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} \right) = \overbrace{\left(\underbrace{\left(\frac{q_{i-1/2}}{\phi \cdot S_{w_i}} \cdot \Delta z \right) \cdot \left(\frac{C_i + C_{i-1}}{2} \right)}_{\text{Advection}} + \underbrace{D_{i-1/2} \cdot \left(\frac{C_i - C_{i-1}}{\Delta z^2} \right)}_{\text{Dispersion}} \right)}^{\text{MassIn}} - \overbrace{\left(\underbrace{\left(\frac{q_{i+1/2}}{\phi \cdot S_{w_i}} \cdot \Delta z \right) \cdot \left(\frac{C_{i+1} + C_i}{2} \right)}_{\text{Advection}} + \underbrace{D_{i+1/2} \cdot \left(\frac{C_{i+1} - C_i}{\Delta z^2} \right)}_{\text{Dispersion}} \right)}^{\text{MassOut}} \quad (\text{A.72})$$

Gathering the similar terms for C_{i-1}^t , C_i^t and C_{i+1}^t yields,

$$C_{i-1} \text{ terms, } \Rightarrow \left(\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{i-1/2}}{\phi \cdot S_{w_i}} \right) - \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i-1/2} \quad (\text{A.73})$$

$$C_i \text{ terms, } \Rightarrow 1 + \left(\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{i-1/2}}{\phi \cdot S_{w_i}} \right) + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i-1/2} - \left(\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{i+1/2}}{\phi \cdot S_{w_i}} \right) + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i+1/2} \quad (\text{A.74})$$

$$C_{i+1} \text{ terms, } \Rightarrow \left(-\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{i+1/2}}{\phi \cdot S_{w_i}} \right) - \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i+1/2} \quad (\text{A.75})$$

And the general equation that needs to be solved is as follows,

$$C_i^{t+\Delta t} = a_1 C_{i-1}^t + a_2 C_i^t + a_3 C_{i+1}^t \quad (\text{A.76})$$

where a_1 , a_2 and a_3 are C_{i-1}^t , C_i^t and C_{i+1}^t terms respectively.

It should be noted that if there are any additional flux terms or source and sink terms, they should be considered as follows,

In case of flux as a source term “i.e. flux in”,

$$C_i^{t+\Delta t} = a_1 C_{i-1}^t + a_2 C_i^t + a_3 C_{i+1}^t + \left(\frac{C_o \cdot q_i \cdot \Delta t}{\phi \cdot S_{w_i} \cdot \Delta z} \right) - R_{s_i} \quad (\text{A.77})$$

where q_i in this case is positive as discussed previously in subsection 3.2.2.2.

In case of flux as a sink term “i.e. flux out”,

$$C_i^{t+\Delta t} = a_1 C_{i-1}^t + a_2 C_i^t + a_3 C_{i+1}^t + \left(\frac{C_i \cdot q_i \cdot \Delta t}{\phi \cdot S_{w_i} \cdot \Delta z} \right) - R_{s_i} \quad (\text{A.78})$$

where q_i in this case is negative to convert the additional flux term to negative sign.

Reader should notice that only for the top grid block, the general equation is slightly different then Eq. (A.72). Eq. (A.79) express the advection and dispersion terms only for the top grid block.

$$\left(\frac{C_n^{t+\Delta t} - C_n^t}{\Delta t} \right) = \overbrace{\left[\left(\frac{q_{n-1/2}}{\phi \cdot S_{w_n} \cdot \Delta z} \right) \cdot \left(\frac{C_n + C_{n-1}}{2} \right) + D_{n-1/2} \cdot \left(\frac{C_n - C_{n-1}}{\Delta z^2} \right) \right]}^{\text{MassIn}} + \left(\frac{\Delta t}{\Delta z} \right) \cdot \left(\frac{Q \cdot C_o}{\phi \cdot S_{w_n}} \right) Q \cdot C_o \quad (\text{A.79})$$

Gathering the similar terms for C_{n-1}^t and C_n^t yields,

$$C_{i-1} \text{ terms, } \Rightarrow \left(\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{n-1/2}}{\phi \cdot S_{w_n}} \right) - \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{n-1/2} \quad (\text{A.80})$$

$$C_i \text{ terms, } \Rightarrow 1 + \left(\frac{\Delta t}{2 \cdot \Delta z} \right) \cdot \left(\frac{q_{n-1/2}}{\phi \cdot S_{w_n}} \right) + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{n-1/2} \quad (\text{A.81})$$

and the general equation that needs to be solved is as follows,

$$C_n^{t+\Delta t} = a_1 C_{n-1}^t + a_2 C_n^t + \left(\frac{\Delta t}{\Delta z} \right) \cdot \left(\frac{Q \cdot C_o}{\phi \cdot S_{w_n}} \right) \quad (\text{A.82})$$

where n expresses the last grid block of the column which is the top of the column.

In this case, there is no C_{n+1}^t as the initial concentration C_o is added as a source term to the equation.

A.9 FINITE DIFFERENCE DERIVATION “UPSTREAM WEIGHTING”

In the upstream weighting, the same concept is used but more weight is considered for the upstream blocks in the direction of the flow. As mentioned in subsection 3.2.3.1, finite difference technique is like the control volume approach. In the control volume approach, one applies mass balance for the advection and dispersion phenomena's on a certain block in the column under study. Fig. (A.2) shows the grid block discretization.

Conducting the mass balance at grid block i shown in Fig. (A.2) yields,

$$\begin{aligned}
\left(\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} \right) = & \overbrace{\left(\underbrace{\left(\frac{q_{i-1/2}}{\phi \cdot S_{w_i} \cdot \Delta z} \right) \cdot C_i}_{\text{Advection}} + \underbrace{D_{i-1/2} \cdot \left(\frac{C_i - C_{i-1}}{\Delta z^2} \right)}_{\text{Dispersion}} \right)}^{\text{MassIn}} - \\
& \overbrace{\left(\underbrace{\left(\frac{q_{i+1/2}}{\phi \cdot S_{w_i} \cdot \Delta z} \right) \cdot C_{i+1}}_{\text{Advection}} + \underbrace{D_{i+1/2} \cdot \left(\frac{C_{i+1} - C_i}{\Delta z^2} \right)}_{\text{Dispersion}} \right)}^{\text{MassOut}}
\end{aligned} \tag{A.83}$$

Gathering the similar terms for C_{i-1}^t , C_i^t and C_{i+1}^t yields,

$$C_{i-1} \text{ terms, } \Rightarrow \left(-\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i-1/2} \tag{A.84}$$

$$C_i \text{ terms, } \Rightarrow 1 + \left(\frac{\Delta t}{\Delta z} \right) \cdot \left(\frac{q_{i-1/2}}{\phi \cdot S_{w_i}} \right) + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i-1/2} + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i+1/2} \tag{A.85}$$

$$C_{i+1} \text{ terms, } \Rightarrow \left(-\frac{\Delta t}{\Delta z^2} \right) \cdot \left(\frac{q_{i+1/2}}{\phi \cdot S_{w_i}} \right) - \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{i+1/2} \tag{A.86}$$

and the general equation that needs to be solved is like the central weighting (Eq. A.76).

As mentioned in the central weighting, the top block has slightly different calculations. The control volume equation for this grid block is as follows,

$$\left(\frac{C_n^{t+\Delta t} - C_n^t}{\Delta t} \right) = \overbrace{\left(\underbrace{\left(\frac{q_{n-1/2}}{\phi \cdot S_{w_n} \cdot \Delta z} \right) \cdot C_n}_{\text{Advection}} + \underbrace{D_{n-1/2} \cdot \left(\frac{C_n - C_{n-1}}{\Delta z^2} \right)}_{\text{Dispersion}} \right)}^{\text{MassIn}} + \left(\frac{\Delta t}{\Delta z} \right) \cdot \left(\frac{Q \cdot C_o}{\phi \cdot S_{w_n}} \right) \tag{A.87}$$

Gathering the similar terms for C_{n-1}^t and C_n^t yields,

$$C_{n-1} \text{ terms, } \Rightarrow \left(-\frac{\Delta t}{\Delta z^2} \right) \cdot D_{n-1/2} \tag{A.88}$$

$$C_n \text{ terms, } \Rightarrow 1 + \left(\frac{\Delta t}{\Delta z} \right) \cdot \left(\frac{q_{n-1/2}}{\phi \cdot S_{w_n}} \right) + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{n-1/2} + \left(\frac{\Delta t}{\Delta z^2} \right) \cdot D_{n+1/2} \quad (\text{A.89})$$

and the general equation that needs to be solved is similar to Eq. (A.82).

A.10 RUNGE-KUTTA METHOD'S MATHEMATICAL EXPLANATION

Runge-Kutta method was named for the German mathematicians Carl Runge (1856-1927) and Wilhelm Kutta (1867-1944) (Edwards and Penney 1985). Basically this method uses Euler method and the improved Euler method with one of the fundamental theorems of calculus known as Simpson's rule to approximate the solution at a new step knowing the solution at the current step. The reader is referred to Edwards and Penney (1985) for further explanation of Euler and improved Euler methods.

For a given function,

$$y' = f(x, y) \quad \text{where } y(x_0) = y_0 \quad (\text{A.90})$$

suppose that we have computed the approximate values $y_1, y_2, \dots, y_n$ and the true values are $g(x_1), g(x_2), \dots, g(x_n)$ and the goal is to calculate $y_{n+1} \approx g(x_{n+1})$. So,

$$g(x_{n+1}) - g(x_n) = \int_{x_n}^{x_{n+1}} g'(x) dx = \int_{x_n}^{x_n+h} g'(x) dx \quad (\text{A.91})$$

where h is the step size and the notation “ ’ ” refers to the derivative of function of interest.

Using Simpson's rule, the integration in Eq. (A.91) yields,

$$g(x_{n+1}) - g(x_n) \approx \frac{h}{6} \left[g'(x_n) + 4g'\left(x_n + \frac{h}{2}\right) + g'(x_{n+1}) \right] \quad (\text{A.92})$$

Then, the new approximated value y_{n+1} can be defined as,

$$y_{n+1} \approx y_n + \frac{h}{6} \left[g'(x_n) + 2g'\left(x_n + \frac{h}{2}\right) + 2g'\left(x_n + \frac{h}{2}\right) + g'(x_{n+1}) \right] \quad (\text{A.93})$$

where the term $4g'(x_n + h/2)$ is going to be split into two terms because of the intention in approximating this slope $g'(x_n + h/2)$ at the mid point $(x_n + h/2)$ of $[x_n, x_{n+1}]$ using two different ways, Euler method and the improved Euler method.

In Eq. (A.93), the actual slopes $g'(x_n)$, $g'(x_n + h/2)$, $g'(x_n + h/2)$ and $g'(x_{n+1})$ are replaced with the following,

$$k_{n1} = f(x_n, y_n) \quad \text{Slope at } x_n \quad (\text{A.94})$$

$$k_{n2} = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_{n1}\right) \quad \text{Slope at the midpoint of } [x_n, x_{n+1}], \text{ using Euler method} \quad (\text{A.95})$$

$$k_{n3} = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_{n2}\right) \quad \text{Slope using the improved Euler method at the midpoint} \quad (\text{A.96})$$

$$k_{n4} = f(x_{n+1}, y_n + hk_{n3}) \quad \text{Slope at } x_{n+1} \text{ using the improved slope } k_{n3} \text{ at the midpoint to step to } x_{n+1} \quad (\text{A.97})$$

and the result of the approximation will be in the form of,

$$y_{n+1} = y_n + \frac{h}{6} [k_{n1} + 2k_{n2} + 2k_{n3} + k_{n4}] \quad (\text{A.98})$$

The previous approximation happens to be equivalent to the five-term (fourth degree) Taylor series expansion which can be describes as,

$$y_{n+1} = y_n + y'_n h + \frac{y''_n}{2!} h^2 + \frac{y^{(3)}_n}{3!} h^3 + \frac{y^{(4)}_n}{4!} h^4 \quad (\text{A.99})$$

A.11 DETAILED CALCULATION FOR THE RELATIVE PERMEABILITY VALUES GIVEN IN TABLES (4.4) AND (4.5)

A spread sheet file was developed to check the theoretical development of the four proposed models. As discussed in chapter 4, the results from the spread sheet file provide an estimate for the relative permeability values. The user can increase the accuracy in the proposed C++ code by dividing the capillary pressure-saturation relationship into more divisions. In this subsection, the spread sheet file will be explained to give an idea of how the relative permeability values were calculated using the three proposed models. The results shown here are the results of using an effective microbial saturation of 0.2 and 0.6 and an effective total saturation of 0.8 (i.e. Tables (4.4) and (4.5) in chapter 4).

First, the spread sheet calculations for effective microbial saturation of 0.2 will be presented with a detailed explanation for the calculation (Table (A.1)) then the effective microbial saturation of 0.6 will be presented later on with the detailed calculations (Table (A.2)).

Table A.1- Spread sheet file for relative permeability calculations using effective microbial saturation of 0.2

Table A.1.1- *Effective total, water and microbial saturations used in the spread sheet file*

S_{em}	0.2	S_{am}	0.1782
S_{et}	0.8	V_m	0.142528
S_{ew}	0.6	m_B	0.333
n	3	m_M	0.667

Table A.1.2- *Relative permeability values for the different models*

	Original	Model #1	Model #2	Model #3
$kr_{Burdine}$	1.36E-01	1.34E-01	2.24E-02	2.18E-02
$kr_{Muallem}$	2.88E-01	2.30E-01	7.20E-02	7.00E-02

Model #3 bottom constant

-2.186

Model #3 top constant

-1.700

Table A.1.3- Input data in the spread sheet file

σ	72.8	dyne/cm
α	0.18	
μ	0.001	Pascal.s
ϕ	0.8	
k_{sat}	0.079	cm/s
γ	9810	N/m ³
θ	0.08736	
ϕ_{free}	0.71	

Table A.1.4- Divisions of the P_c – Sat. curve

Divisions	Sat.
4	0.125
	0.375
	0.625
	0.875

Table A.1.5- Capillary tubes area check

radius check		
if $th < r_i$	1	safe
if $th \geq r_i$	0	clogged

Table A.1.6- Filled volume for the given saturations

V_1	0.17816	V_{m1}	0.142528
V_2	0.17816	V_{m2}	0
V_3	0.17816	V_{m3}	0
V_4	0.17816	V_{m4}	0
V_{total}	0.71		

Table A.1.7- Model #3 calculations

Model 3 calculations							new th 0.00198
#	Pc's	Pc's in dyne/cm ²	r's	# of Tubes	Sum of r's ⁴	Check Tubes Area	Sum of (r's $\cdot th$) ⁴
1	15.479	14984.03313	0.00972	600.6134186	5.35E-06	1	2.16E-06
2	8.317	8050.870561	0.01809	173.3896899	1.85E-05	1	1.17E-05
3	5.599	5420.512796	0.02686	78.59923686	4.09E-05	1	3.01E-05
4	3.363	3255.306988	0.04473	28.34793853	0.000113	1	9.50E-05
					0.0001783		0.000139

Table A.1.8- Biofilm thickness calculations

Model 3 calculations		th value		Condition
Sum (# of Tubes)	Sum (# of Tubes * r)	Tube #	-ve	
880.9502839	12.3510849	1	0.00198	0.00198
280.3368653	6.51491829	2	0.00000	0.00000
106.9471754	3.37916562	3	0.00000	0.00000
28.34793853	1.26791724	4	0.00000	0.00000

In the spread sheet file, Table (A.1.2) shows the values of the relative permeability show in chapter 4 Table (4.4). The original values are calculated as follows,

For Burdine,
$$k_r = (0.8)^2 \cdot (1 - (1 - 0.8^{1/0.333})^{0.333}) = 1.36 \times 10^{-01}$$

For Mualem,
$$k_r = (0.8)^{1/2} \cdot (1 - (1 - 0.8^{1/0.667})^{0.667})^2 = 2.88 \times 10^{-01}$$

When the effective microbial saturation reaches 0.2, the relative permeability values predicted with the three proposed models are calculated as follows:

A.11.1 MODEL # 1 WITH EFFECTIVE MICROBIAL SATURATION OF 0.2

Using Eq. (4.4) or Eq. (4.5), the relative permeability value is as follows,

$$\text{For Burdine, } k_r = (0.8)^2 \cdot ((1 - 0.2^{1/0.333})^{0.333} - (1 - 0.8^{1/0.333})^{0.333}) = 1.34 \times 10^{-02}$$

$$\text{For Mualem, } k_r = (0.8)^{1/2} \cdot ((1 - 0.2^{1/0.667})^{0.667} - (1 - 0.8^{1/0.667})^{0.667})^2 = 2.30 \times 10^{-02}$$

A.11.2 MODEL # 2 WITH EFFECTIVE MICROBIAL SATURATION OF 0.2

Using Eq. (4.6) or Eq. (4.7), the relative permeability value is as follows,

$$\text{For Burdine, } k_r = (0.6)^2 \cdot (1 - (1 - 0.6^{1/0.333})^{0.333}) \cdot (1 - 0.2) = 2.24 \times 10^{-02}$$

$$\text{For Mualem, } k_r = (0.6)^{1/2} \cdot (1 - (1 - 0.6^{1/0.667})^{0.667})^2 \cdot (1 - 0.2) = 7.20 \times 10^{-02}$$

A.11.3 MODEL # 3 WITH EFFECTIVE MICROBIAL SATURATION OF 0.2

Table (A.1.3) summarizes the assumed data used in the calculations of Model #3.

The capillary pressure–saturation relationship is divided into 4-divisions (Table (A.1.4))

Capillary pressure values for the given 4-divisions can be calculated using Eq. (4.8) as follows (Table (A.1.7)),

$$P_{c1} = \frac{((0.125)^{-1/0.667} - 1)^{\left(\frac{1}{3.0}\right)}}{0.18} = 15.479 \text{ cm} = 14984.033 \text{ dyne/cm}$$

$$P_{c2} = \frac{((0.375)^{-1/0.667} - 1)^{\left(\frac{1}{3.0}\right)}}{0.18} = 8.317 \text{ cm} = 8050.871 \text{ dyne/cm}$$

$$P_{c3} = \frac{\left((0.625)^{-1/0.667} - 1\right)^{\left(\frac{1}{3.0}\right)}}{0.18} = 5.599 \text{ cm} = \mathbf{5420.513 \text{ dyne/cm}}$$

$$P_{c4} = \frac{\left((0.875)^{-1/0.667} - 1\right)^{\left(\frac{1}{3.0}\right)}}{0.18} = 3.363 \text{ cm} = \mathbf{3255.307 \text{ dyne/cm}}$$

Then, the radii can be calculated using Eq. (3.1) after rearranging as follows,

$$r_1 = \frac{(2)(74.0)}{(14984.033)} = \mathbf{0.00972 \text{ cm}}$$

$$r_2 = \mathbf{0.01809 \text{ cm}}$$

$$r_3 = \mathbf{0.02686 \text{ cm}}$$

$$r_4 = \mathbf{0.04473 \text{ cm}}$$

The number of capillary tubes will be,

$$\# \text{ of Tubes}_1 = \frac{0.71}{(4)(\pi)(0.00972)^2} = \mathbf{600.613 \text{ tubes}}$$

$$\# \text{ of Tubes}_2 = \mathbf{173.390 \text{ tubes}}$$

$$\# \text{ of Tubes}_3 = \mathbf{78.599 \text{ tubes}}$$

$$\# \text{ of Tubes}_4 = \mathbf{28.348 \text{ tubes}}$$

The new proposed constant $U_o|_0^{Porosity}$ can then be calculated using Eq. (4.13) as follows,

$$U_o|_0^{Porosity} = \left(-\frac{(0.0001783)}{8} \cdot \frac{9810}{0.001} \right) = \mathbf{-2.186}$$

By assuming an effective microbial saturation of 0.6, the actual microbial saturation will be as follows,

$$S_{am} = 0.2 (1 - 0.08736/ 0.8) = \mathbf{0.1782}$$

Then,

$$\mathbf{Microbial\ volume\ (V_m) = (0.1782) (0.8) = 0.1426\ cm^3}$$

This microbial volume will be distributed overall the radii. The biofilm thickness (th) at this time can be calculated using Eq. (4.9). and the quadratic equation that need to be solve is as follows,

$$\begin{aligned} & \left(\#of\ Tubes_1 \cdot \pi \cdot r_1^2 - \#of\ Tubes_1 \cdot \pi \cdot (r_1 - th)^2 \right) + \left(\#of\ Tubes_2 \cdot \pi \cdot r_2^2 - \#of\ Tubes_2 \cdot \pi \cdot (r_2 - th)^2 \right) \\ & + \\ & \left(\#of\ Tubes_3 \cdot \pi \cdot r_3^2 - \#of\ Tubes_3 \cdot \pi \cdot (r_3 - th)^2 \right) + \left(\#of\ Tubes_4 \cdot \pi \cdot r_4^2 - \#of\ Tubes_4 \cdot \pi \cdot (r_4 - th)^2 \right) \\ & = V_m \end{aligned}$$

and with rearranging becomes,

$$\begin{aligned} & th^2 \cdot (\#of\ Tubes_1 + \#of\ Tubes_2 + \#of\ Tubes_3 + \#of\ Tubes_4) - \\ & 2 \cdot th \cdot (\#of\ Tubes_1 \cdot r_1 + \#of\ Tubes_2 \cdot r_2 + \#of\ Tubes_3 \cdot r_3 + \#of\ Tubes_4 \cdot r_4) \\ & + \frac{New\ microbial\ volume}{\pi} = 0.0 \end{aligned}$$

Numerically,

$$\begin{aligned} & (th^2)(600.613 + 173.390 + 78.599 + 28.348) - (2)(th)[(600.613)(0.00972) + \\ & (173.390)(0.01809) + (78.599)(0.02686) + (28.348)(0.04473)] + \frac{0.142528}{\pi} = 0.0 \end{aligned}$$

By solving this equation, the biofilm thickness will be,

$$th = 0.00198 \text{ cm}$$

Since the thickness of the biofilm is a positive real value, hence the present microbial value will not clog any of the pores. Reader should be noted that if the result of the biofilm thickness is a negative or a complex value, this means that some pores are already clogged and have to be excluded from the biofilm thickness calculation. In addition a new microbial volume has to be calculated to exclude the equivalent volume of microbars that clogged the excluded pores.

The constant proposed with Eq. (4.14) can be calculated as,

$$U_i|_0^{Porosity} = \left(-\frac{(0.000139)}{8} \cdot \frac{9810}{0.001} \right) = -1.700$$

Finally, the relative permeability value for Burdine or Mualem can be obtained using Eq. (4.15) and (4.16) respectively as follows,

$$\text{For Burdine, } k_r = (0.6)^2 \cdot (1 - (1 - 0.6^{1/0.333})^{0.333}) \cdot \frac{-1.700}{-2.186} = 2.18 \times 10^{-02}$$

$$\text{For Mualem, } k_r = (0.6)^{1/2} \cdot (1 - (1 - 0.6^{1/0.667})^{0.667})^2 \cdot \frac{-1.700}{-2.186} = 7.00 \times 10^{-02}$$

Table A.2- Spread sheet file for relative permeability calculations using effective microbial saturation of 0.6

Table A.2.1- Effective total, water and microbial saturations used in the spread sheet file

S_{em}	0.6	S_{am}	0.5345
S_{et}	0.8	V_m	0.427584
S_{ew}	0.2	m_B	0.333
n	3	m_M	0.667

Table A.2.2- Relative permeability values for the different models

	Original	Model #1	Model #2	Model #3
$kr_{Burdine}$	1.36E-01	8.63E-02	4.28E-05	4.04E-05
kr_{Muskem}	2.88E-01	4.60E-02	6.56E-04	6.20E-04

Model #3 bottom constant

-2.186

Model #3 top constant

-0.826

Table A.2.3- Input data in the spread sheet file

σ	72.8	dyne/cm
α	0.18	
μ	0.001	Pascal.s
ϕ	0.8	
$ksat$	0.079	cm/s
γ	9810	N/m ³
θ	0.08736	
ϕ_{free}	0.71	

Table A.2.4- Divisions of the P_c – Sat. curve

Divisions	Sat.
4	0.125
	0.375
	0.625
	0.875

Table A.2.5- Capillary tubes area check

radius check		
if $th < r_1$	1	safe
if $th \geq r_1$	0	clogged

Table A.2.6- Filled volume for the given saturations

V_1	0.17816	V_{m1}	0.427584
V_2	0.17816	V_{m2}	0.249424
V_3	0.17816	V_{m3}	0.071264
V_4	0.17816	V_{m4}	0
V_{total}	0.71		

Table A.2.7- Model #3 calculations

Model # 3 calculations							new th 0.00356
#	Pc's	Pc's in dyne/cm ²	r's	# of Tubes	Sum of r's ⁴	Check Tubes Area	Sum of (r's-th) ⁴
1	15.479	14984.03313	0.00972	600.613	5.35E-06	1	1.36E-05
2	8.317	8050.870561	0.01809	173.390	1.85E-05	1	2.15E-05
3	5.599	5420.512796	0.02686	78.599	4.09E-05	1	1.10E-05
4	3.363	3255.306988	0.04473	28.348	0.000113	1	5.42E-05
					0.0001783		2.32E-05

Table A.2.8- Biofilm thickness calculations

Model #3 calculations		Tube #	th value		Condition
Sum (# of Tubes)	Sum (# of Tubes * r)		-ve	+ve	
880.950	12.351	1	0.00753	0.00000	0.00753
280.337	6.515	2	0.00721	0.00000	0.00721
106.947	3.379	3	0.00356	0.05964	0.00356
28.348	1.268	4	0.00000	0.00000	0.00000

In the spread sheet file, Table (A.2.2) shows the values of the relative permeability show in chapter 4 Table (4.5). The original values are calculated as follows,

For Burdine,
$$k_r = (0.8)^2 \cdot (1 - (1 - 0.8^{1/0.333})^{0.333}) = 1.36 \times 10^{-01}$$

For Mualem,
$$k_r = (0.8)^{1/2} \cdot (1 - (1 - 0.8^{1/0.667})^{0.667})^2 = 2.88 \times 10^{-01}$$

When the effective microbial saturation reaches 0.6, the relative permeability values predicted with the three proposed models are calculated as follows:

A.11.4 MODEL # 1 WITH EFFECTIVE MICROBIAL SATURATION OF 0.6

Using Eq. (4.4) or Eq. (4.5), the relative permeability value is as follows,

For Burdine,
$$k_r = (0.8)^2 \cdot ((1 - 0.6^{1/0.333})^{0.333} - (1 - 0.8^{1/0.333})^{0.333}) = 8.63 \times 10^{-02}$$

For Mualem,
$$k_r = (0.8)^{1/2} \cdot ((1 - 0.6^{1/0.667})^{0.667} - (1 - 0.8^{1/0.667})^{0.667})^2 = 4.60 \times 10^{-02}$$

A.11.5 MODEL # 2 WITH EFFECTIVE MICROBIAL SATURATION OF 0.6

Using Eq. (4.6) or Eq. (4.7), the relative permeability value is as follows,

For Burdine,
$$k_r = (0.2)^2 \cdot (1 - (1 - 0.2^{1/0.333})^{0.333}) \cdot (1 - 0.6) = 4.28 \times 10^{-05}$$

For Mualem,
$$k_r = (0.2)^{1/2} \cdot (1 - (1 - 0.2^{1/0.667})^{0.667})^2 \cdot (1 - 0.6) = 6.56 \times 10^{-04}$$

A.11.6 MODEL # 3 WITH EFFECTIVE MICROBIAL SATURATION OF 0.6

Table (A.2.3) summarizes the assumed data used in the calculations of Model #3. The capillary pressure–saturation relationship is divided into 4-divisions (Table (A.2.4))

Capillary pressure values, pores radii of the capillary tubes and the number of capillary tubes can be calculated as previously discussed in subsection A.11.3.

By assuming an effective microbial saturation of 0.6, the actual microbial saturation will be as follows,

$$S_{am} = 0.6 (1 - 0.08736/ 0.8) = \mathbf{0.5345}$$

Then,

$$\mathbf{Microbial\ volume\ (V_m) = (0.5345) (0.8) = 0.4276\ cm^3}$$

Numerically, the biofilm thickness can be calculated as follows,

$$(th^2)(600.613 + 173.390 + 78.599 + 28.348) - (2)(th)[(600.613)(0.00972) + (173.390)(0.01809) + (78.599)(0.02686) + (28.348)(0.04473)] + \frac{0.07126}{\pi} = 0.0$$

By solving this equation, the biofilm thickness will be,

$$\mathbf{th = 0.00753\ cm}$$

The constant proposed with Eq. (4.14) can be calculated as,

$$U_i \Big|_0^{Porosity} = \left(-\frac{(6.737E-05)}{8} \cdot \frac{\frac{9810}{100}}{0.001} \right) = \mathbf{-0.826}$$

Finally, the relative permeability value for Burdine or Mualem can be obtained using Eq. (4.15) and (4.16) respectively as follows,

$$\text{For Burdine, } \mathbf{k_r} = (0.2)^2 \cdot (1 - (1 - 0.2^{1/0.333})^{0.333}) \cdot \frac{-0.826}{-2.186} = \mathbf{4.04 \times 10^{-05}}$$

$$\text{For Mualem, } \mathbf{k_r} = (0.2)^{1/2} \cdot (1 - (1 - 0.2^{1/0.667})^{0.667})^2 \cdot \frac{-0.826}{-2.186} = \mathbf{6.20 \times 10^{-04}}$$

APPENDIX B – FLOW CHARTS

The proposed code contains eleven functions, a main function and ten other different functions used to calculate different variables in the main function.

The Main function is the main code body. This function as shown in Flow Chart (1) is used to solve the flow equation first then the contaminant transport equation using the chosen sink term according to the user interest. Description of the main function is shown in Flow Chart (4).

The main functions reads from a regular text file, “Input.txt”, which contains data for time and distance discretization, soil type, dispersivity value, van Genuchten parameters and the initial and boundary conditions for flow and substrate added. The input file also contains data for the sink term used whether it is first order or Monod kinetics. A sample of input file is shown in Appendix C. In Flow Chart (4), the “Local input” are additional variables used in the main body of the code for calculation purposes and the “Variable Initialization” holds other processes like conversions factors. The output file of the main function will be described in Appendix C.

The other ten functions read their input data from the main function as follows:

B.1 “FUNCTION” USED TO CALCULATE HEADS

The input data for this function are time and distance discretization, soil porosity, actual water saturation at the current and previous time steps, saturated hydraulic conductivity at the interface of the blocks, total head, relative permeability at the

interface of the blocks, prescribes flux, top and bottom boundary conditions and the total number of blocks. Description of this function is shown in Flow Chart (5).

B.2 SATURATION FUNCTION

The input data for this function are the capillary pressures calculated earlier in the main function, van Genuchten parameters, soil porosity, irreducible moisture content, effective microbial saturation and the microbial growth method used “i.e. Burdine or Mualem”. Description of this function is shown in Flow Chart (6). This function returns the actual total saturation.

B.3 RELATIVE PERMEABILITY FUNCTION FOR THE FIRST AND SECOND PROPOSED SCENARIOS

The input data for this function are van Genuchten parameters, soil porosity, irreducible moisture content, effective and total microbial saturations and the microbial growth method used “i.e. Burdine or Mualem”. Description of this function is shown in Flow Chart (7). This function returns the relative permeability.

B.4 RELATIVE PERMEABILITY FUNCTION FOR THE THIRD PROPOSED SCENARIO

The input data for this function are van Genuchten parameters, soil porosity, time and distance discretization, effective total and microbial saturations, the microbial growth

method used “i.e. Burdine or Mualem”, surface tension for water/air interface, viscosity of water, specific gravity of water and microbial volume calculated earlier in the main function. Description of this function is shown in Flow Chart (8). This function returns the relative permeability and saves other parameters like number and radius of capillary tubes.

B.5 FLUID MASS BALANCE FUNCTION

The input data for this function are top and bottom boundary conditions, saturated hydraulic conductivity, relative permeability, actual water saturation, soil porosity, time and distance discretization, initial water moisture content and area under the concentration versus distance curve for the previous time step. Description of this function is shown in Flow Chart (9). This function returns the terms used in Eq. (3.49) and saves other parameters to use it later in the cumulative fluid mass balance function.

B.6 CONTAMINANT MASS BALANCE FUNCTION

The input data for this function are almost the same as the fluid mass balance function. In addition to that, this function takes the concentration and Monod Kinetics parameters or first order decay for the sink term. Description of this function is shown in Flow Chart (10). This function returns the terms used in Eq. (3.56) and saves other parameters to use it later in the cumulative contaminant mass balance function.

B.7 CUMULATIVE FLUID MASS BALANCE FUNCTION

The input data for this function are the cumulative flux added to the system, cumulative flow out of the system and storage over the entire simulation time. Description of this function is shown in Flow Chart (2). This function returns the cumulative fluid mass balance for the whole simulation.

B.8 CUMULATIVE CONTAMINANT MASS BALANCE FUNCTION

The input data for this function are the cumulative mass in, cumulative mass out, storage over the entire simulation time and the cumulative degradation. Description of this function is shown in Flow Chart (3). This function returns the cumulative contaminant mass balance for the whole simulation.

B.9 COMPARE FUNCTION

This function is used to check if the desired solutions for the total heads reached or more iterations should be conduct. Description of this function is shown in Flow Chart (11). This function returns true or false for whether other iteration should be conduct.

B.10 TIME TOLERANCE FUNCTION

This function is used for printing. It compares the printing time with the current time and it returns true or false for whether printing time is reached or not. Description of this function is shown in Flow Chart (12).

Flow Chart B.1- Global Over View

Flow Chart B.2- Cumulative Fluid Mass Balance Function

Flow Chart B.3- Cumulative Contaminant Mass Balance Function

Flow Chart B.4- Main Function

Flow Chart B.5- "Function" To Calculate Heads

Flow Chart B.6- Saturation Function

Flow Chart B.7- Relative Permeability for the First and Second Scenario

Flow Chart B.8- Relative Permeability for the Third Scenario

Flow Chart B.9- Fluid Mass Balance Function

Flow Chart B.10- Contaminant Mass Balance Function

Flow Chart B.11- Compare Function

Flow Chart B.12- Time Tolerance Function

APPENDIX C – USER’S GUIDE FOR INPUT FILE

C.1 INPUT FILE FOR FLOW AND CONTAMINANT TRANSPORT BUT WITHOUT SINK TERM AND WITH CONTINUOUS LOADING

1	50	Grid size (cm), number of blocks
1	180000 3600	Time step size (s), maximum time for simulation, print every 3600 s
	0.00428	Saturated hydraulic conductivity (cm/s)
	0.312	Porosity
	0.0265	Irreducible water content
2.2	0.044	Van Genuchten parameters, n and alpha (cm ⁻¹)
1	0.00001	Dispersivity (cm), Molecular diffusion (cm ² /s)
First order decay rate’s parameter		
t	-0.000574	t for first order decay rate, the value of the T _{1/2} in years and enter any –ve number if no decay rate
Monod Kinetic’s parameters		
R	-500	R for Monod kinetics, Value of Runge-Kutta steps and enter any – ve number for no Monod kinetics
B		Conductivity model using Burdine if "B" or Mualem if "M"
1		Model used to calculate relative permeability term, 1 for Model #1, 2 for #2 and 3 for #3
2		Number of stress periods
	-9.9	Initial total head of the column (cm)
N		Loading condition, P for Pulse and N for Continuous
	10800	First stress period from time zero to 10800 s
W H		B.C. at the top of the column is flux for “W”, B.C. at the bottom of the column is head for “H”
	0.00231	Flux B.C. value at the top of the column during the first stress period (cm/s)
	-9.9	Head B.C. value at the bottom of the column during the first stress period (cm)
U		Weighting used for the contaminant transport equation during the first stress period “U for Upstream Weighting”

0.0	Initial substrate concentration at the top boundary during the first stress period (mg/L)			
0.0	0.0	0.0	0.0	Additional flux values at any level of the column. positive if source and negative if sink
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
0.0	0.0	0.0	0.0	
180000	Second stress period from time (10800 + Δ t) to 180000 s			
W	H	B.C. at the top of the column is flux for “W”, B.C. at the bottom of the column is head for “H”		
0.00231	Flux B.C. value at the top of the column during the second stress period (cm/s)			
-9.9	Head B.C. value at the bottom of the column during the second stress period (cm)			
C	Weighting used for the contaminant transport equation during the second stress period “U for Central Weighting”			
2000.0	Initial substrate concentration at the top boundary during the second stress period (mg/L)			
	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

Only the text not in bold is used in the input file, the bold text is only for explanation and Not to be used in the input file.

C.2 INPUT FILE FOR FLOW AND CONTAMINANT TRANSPORT WITH FIRST ORDER DECAY RATE AS SINK TERM AND CONTINUOUS LOADING

1 100
1 180000 3600
0.00428
0.312
0.0265
2.2 0.044
1 0.00001

t 0.000574

t for first order decay rate, the value of the $T_{1/2}$ in years and enter any -ve number if no decay rate

R -500

M

3

Model used to calculate relative permeability term, 1 for Model #1, 2 for #2 and 3 for #3

20

Number of divisions

72.8

Surface tension for water/air interface (dyne/cm)

9810

Specific gravity of water (N/m^3) or (Pascal/m)

0.001

Viscosity of water (Pascal. s)

2

-9.9

N

10800

W H

0.00231

-9.9

U

0.0

0.0 0.0 0.0 0.0

C.3 INPUT FILE FOR FLOW AND CONTAMINANT TRANSPORT WITH MONOD KINETICS AS SINK TERM AND PULSE LOADING

1 100
 1 172800 3600
 0.00428
 0.312
 0.0265
 2.2 0.044
 1 0.00001

 t -0.000574

Monod Kinetic's parameters

R 100 R for Monod kinetics, value of Runge-Kutta steps
 0.678 Y, the cell yield coefficient (mg cells/ mg BOD)
 0.00004861 q_m , the maximum specified rate of substrate utilization (mg BOD /
 mg cells . s)
 0.00000081 B, the cell decay coefficient (s^{-1})
 1 M_{T0} , the initial microbial concentration (mg/L)
 0.218 K_s , the half-velocity constant (mg/L)
 1.39 ρ , dry bacteria density in (gm/cm^3)

B

1

2

-9.9

P

900	W	H	0.022222	-9.9	U	2000.0
43200	W	H	0.000000	-9.9	U	0.0
44100	W	H	0.022222	-9.9	U	2000.0
86400	W	H	0.000000	-9.9	U	0.0
87300	W	H	0.022222	-9.9	U	2000.0
129600	W	H	0.000000	-9.9	U	0.0
130500	W	H	0.022222	-9.9	U	2000.0
172800	W	H	0.000000	-9.9	U	0.0