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# Simplified Modelling of Pollutant Transport in Naturally-layered Aquifers



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## Abstract

Chemical species such as tracers or dissolved pollutants flow along with the slow-moving water as it makes its way through the complex porous structure of the aquifer; during this process they are dispersed in different directions. The rate of dispersion depends on the geometric characteristics of the porous structure and speed of the fluid.

Generally, groundwater systems have layered structures determined by different events in the geological processes that formed them. The layers in a system have different physical properties, and their thicknesses are not uniform. This naturally layered structure is used here to advantage by discretizing them into almost horizontal layers, where each may have different geometrical characteristics such as thickness permeability, dispersivity, porosity, etc. The system of advection-dispersion equations that model the fluid and species transport then have coefficients that depend mainly on depth, but with a layer composition that may change with horizontal distance.

The mean dynamic pressure (or mean hydraulic head) may be assumed constant vertically at each horizontal point if it is not in the vicinity of a well or where there is very small vertical flow. In the vicinity of recharge or pumping wells, the mean dynamic pressures or hydraulic heads for each sub-layer of the aquifer may be allowed to have different values for each different sub-layer. Steady-state fluid flow is considered in this thesis in both confined and phreatic (unconfined) aquifers.

This thesis work is dedicated to my father, Farman Ali, who has been a constant source of support and encouragement during the challenges of graduate school and life. I am truly thankful for having you in my life.

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# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Background</b>	<b>7</b>
<b>3</b>	<b>Fluid Flow Model for a Confined Aquifer</b>	<b>13</b>
3.1	Fluid flow in absence of wells . . . . .	13
3.1.1	Illustration . . . . .	17
3.2	Flow in presence of recharge or pumping well across the aquifer thickness	18
3.2.1	Illustration: analytic solution of a very special case . . . . .	20
3.2.2	Illustration: a two-dimensional single-layered (homogeneous) aquifer with a recharge well . . . . .	21
3.2.3	Illustration: both recharge and pumping wells in two-dimensional aquifer . . . . .	23
3.3	Flow in a layered aquifer with a point source . . . . .	24
3.3.1	Illustration: point fluid source in one sub-layer . . . . .	26
3.3.2	Distributed fluid source at the surface . . . . .	27
<b>4</b>	<b>Fluid Flow Model for a Phreatic Aquifer</b>	<b>31</b>
4.1	Fluid flow in absence of wells . . . . .	31
4.1.1	Analytic solution for a special case of a non-homogeneous aquifer	33
4.1.2	A one-dimensional phreatic aquifer with $K$ as a function of $x$ . .	36
4.1.3	A lens in a phreatic aquifer . . . . .	37
4.2	Phreatic aquifer with pumping or recharge well across the aquifer thickness	39
4.2.1	Analytic solution for a special case . . . . .	39
4.2.2	Analytic solution for a special case of pumping well . . . . .	39

## CONTENTS

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4.3	Multi-layered phreatic aquifer with pumping or recharge in one of the sub-layers . . . . .	41
4.3.1	Point recharge well in a sub-layer . . . . .	43
4.3.2	Transverse running stream in the top sub-layer . . . . .	44
<b>5</b>	<b>Pollutant Transport in Steady Fluid Flow</b>	<b>49</b>
5.1	Conceptual model . . . . .	50
5.2	Illustrations: confined aquifers . . . . .	54
5.2.1	Homogeneous aquifers . . . . .	54
5.2.2	One-dimensional multi-layered aquifers . . . . .	63
5.2.3	Signalled sources . . . . .	67
5.2.4	Layered aquifer with a point pollutant source with negligible fluid recharge . . . . .	67
5.2.5	A lens in a confined aquifer . . . . .	69
5.2.6	Point source of contaminated fluid in one sub-layer . . . . .	73
5.2.7	A stream of contaminated water at the surface . . . . .	73
5.3	Illustrations: phreatic aquifers . . . . .	74
5.3.1	Effect of varying bottom surface in a homogeneous aquifer . . . . .	74
5.3.2	A lens in a phreatic aquifer . . . . .	76
5.3.3	A point source of contaminated fluid in one sub-layer . . . . .	80
5.3.4	Contaminated stream at the top . . . . .	80
5.4	Site data . . . . .	83
<b>6</b>	<b>Pollutant Remediation</b>	<b>85</b>
6.1	One-dimensional homogeneous aquifers . . . . .	86
6.1.1	Illustration . . . . .	87
6.2	Two-dimensional homogeneous aquifers . . . . .	89
6.2.1	Illustration . . . . .	90
6.3	Multi-layered aquifers . . . . .	93
6.3.1	Illustration . . . . .	94
6.4	Location of oxidizer release to achieve optimum remediation . . . . .	96

<b>7 Summary and Discussion</b>	<b>101</b>
7.1 Summary . . . . .	101
7.2 Further research . . . . .	103
7.3 Publications and presentations . . . . .	103
<b>References</b>	<b>105</b>





# Nomenclature

- $\bar{c}$  average concentration of pollutant in the fluid averaged over sub-layer thickness [ $\text{kg m}^{-3}$ ]
- D** three-dimensional tensor coefficient of mechanical dispersion of a dissolved pollutant while it flows in the porous media [ $\text{m}^2 \text{s}^{-1}$ ]
- $D$  scalar coefficient of mechanical dispersion of a dissolved pollutant while it flows in the porous media [ $\text{m}^2 \text{s}^{-1}$ ]
- $F$  steady rate of fluid recharge in or pumping out of a sub-layer of the aquifer ( $F$  has dimensions of [ $\text{m s}^{-1}$ ] when thickness varies in one horizontal direction and of [ $\text{m}^2 \text{s}^{-1}$ ] when thickness varies in both horizontal directions)
- $f$  mass flux function in a sub-layer of the aquifer or fluid recharge flux function in or pumping flux function out of a sub-layer of the aquifer (if  $f$  is used for mass flux of a chemical, it has dimensions of [ $\text{kg m}^{-3} \text{s}^{-1}$ ] and if it is used for fluid flux it has dimensions of [ $\text{s}^{-1}$ ])
- $g$  gravitational acceleration [ $\text{m s}^{-2}$ ]
- $H$  hydraulic head [m]
- $\bar{H}$  mean hydraulic head averaged over the sub-layer thickness [m]
- $h$  thickness of the sub-layer or the aquifer [m]
- K** permeability tensor of the porous media [ $\text{m}^2$ ]
- $K$  isotropic permeability of the porous media [ $\text{m}^2$ ]

## CONTENTS

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- $\bar{K}$  mean (weighted) isotropic permeability of the aquifer averaged over the aquifer thickness, i.e.,  $\bar{K} = (\sum h_i K_i) / h$  [ $\text{m}^2$ ]
- $M$  steady mass flux of fluid in or out of a sub-layer of the aquifer [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
- $P$  dynamic pressure of the fluid [ $\text{kg m}^{-1} \text{s}^{-2}$ ]
- $\bar{P}$  mean dynamic pressure of the fluid averaged over the sub-layer thickness [ $\text{kg m}^{-1} \text{s}^{-2}$ ]
- $p$  absolute pressure of the fluid [ $\text{kg m}^{-1} \text{s}^{-2}$ ]
- $Q$  instantaneous flow of mass in a sub-layer of the aquifer ( $Q$  has dimensions of [ $\text{kg m}^{-2}$ ] when thickness varies in one horizontal direction and of [ $\text{kg m}^{-1}$ ] when thickness varies in both horizontal directions)
- $\mathbf{q}$  total horizontal volume flux  $\mathbf{q} = (q_x, q_y)$  through the whole aquifer [ $\text{m}^2 \text{s}^{-1}$ ]
- $q$  steady mass or volume flux of fluid or a chemical in a sub-layer of the aquifer (if  $q$  is used for mass flux of a chemical, it has dimensions of [ $\text{kg m}^{-2} \text{s}^{-1}$ ] when thickness varies in one horizontal direction and [ $\text{kg m}^{-1} \text{s}^{-1}$ ] when thickness varies in both horizontal directions and if  $q$  is used for the fluid flux, it has dimensions of [ $\text{m s}^{-1}$ ] when thickness varies in one horizontal direction and [ $\text{m}^2 \text{s}^{-1}$ ] when thickness varies in both horizontal directions)
- $r$  the fluid flux normal to the layer interface from the lower sub-layer to the upper sub-layer [ $\text{m s}^{-1}$ ]
- $\mathbf{u}$  Darcy velocity vector of fluid  $\mathbf{u} = (u, v, w)$  in the porous media [ $\text{m s}^{-1}$ ]
- $\bar{\mathbf{u}}$  average two-dimensional horizontal Darcy velocity vector of fluid  $\bar{\mathbf{u}} = (\bar{u}, \bar{v})$  in the porous media averaged over sub-layer thickness [ $\text{m s}^{-1}$ ]
- $z$  height above datum [ $\text{m}$ ]

## Greek Symbols

- $\alpha$  dispersivity of the porous medium [ $\text{m}$ ]

$\delta$	Dirac delta function
$\kappa$	hydraulic conductivity [ $\text{m s}^{-1}$ ]
$\mu$	dynamic viscosity of the fluid [ $\text{kg m}^{-1} \text{s}^{-1}$ ]
$\rho$	density of the fluid [ $\text{kg m}^{-3}$ ]
$\tau$	interlayer dispersive transfer coefficient [ $\text{m s}^{-1}$ ]
$\Phi$	the function $\Phi_i$ for the $i$ th interface level between the sub-layers (starting from bottom) is defined by $\Phi_i(x, y, z) = z - z_i(x, y)$ , where $z_i$ is the interface level between the $i - 1$ th and the $i$ th sub-layers [m]
$\phi$	porosity of the porous media [-]
$\psi$	the two-dimensional stream function [ $\text{m}^3 \text{s}^{-1}$ ]

### Subscripts

<i>atm</i>	atmospheric
<i>d</i>	downstream
<i>I</i>	injection
<i>L</i>	longitudinal
<i>P</i>	pollutant
<i>R</i>	remediating agent
<i>ret</i>	retention
<i>s</i>	curve along phreatic surface
<i>st</i>	stream
<i>T</i>	transverse
<i>t</i>	top
<i>tot</i>	total
<i>u</i>	upstream
<i>V</i>	volume
<i>W</i>	withdrawal
<i>x, y, z</i>	principal directions of Cartesian coordinate system