

Copyright is owned by the Author of the thesis. Permission is given for a copy to be downloaded by an individual for the purpose of research and private study only. The thesis may not be reproduced elsewhere without the permission of the Author.

SOLUTE TRANSPORT IN A LAYERED FIELD SOIL

A thesis presented in partial fulfilment of the requirements
for the degree of
Doctor of Philosophy
in
Soil Science
at Massey University

Valerie Olga Snow

1992

Massey University Library
Thesis Copyright Form

Title of thesis: *Solute Transport in a Layered Field Soil*

(1) (a) I give permission for my thesis to be made available to readers in Massey University Library under conditions determined by the Librarian.

~~(b) I do not wish my thesis to be made available to readers without my written consent for ... months.~~

(2) (a) I agree that my thesis, or a copy, may be sent to another institution under conditions determined by the Librarian.

~~(b) I do not wish my thesis, or a copy, to be sent to another institution without my written consent for ... months.~~

(3) (a) I agree that my thesis may be copied for Library use.

~~(b) I do not wish my thesis to be copied for Library use for ... months.~~

Signed

Snow
A. Snow

Date

17/2/92

The copyright of this thesis belongs to the author. Readers must sign their name in the space below to show that they recognise this. They are asked to add their permanent address.

NAME AND ADDRESS

DATE

ABSTRACT

Although concern about the effects of movement of chemicals through soil has brought about a need for greater understanding of solute transport, the question as to where best to focus the research effort remains open.

Initially a philosophical framework was presented that described in a general sense how research into solute transport has been conducted. It was argued that we must combine modelling with experimentation for effective progress in understanding, and that the efforts in field versus lab experimentation and process- versus non-mechanistic modelling should be balanced. Currently there is a need for more field experimentation, but the preferred direction of the modelling effort is less clear. Both process-based and non-mechanistic models are considered in order to deduce the effect of soil layering on solute transport.

Field experiments were carried out on a soil consisting of three layers of distinct texture. This soil was instrumented with porous cup samplers at four depths at twenty sites. There was also a 2 m² lysimeter within the plot.

In the first experiment irrigation was used to supplement rainfall in order to leach a surface application of solid KCl through the soil. Porous cup samples of the soil solution were collected on numerous occasions and soil cores less often. The experiment of the following year was similar in design except that no irrigation was used. Finally, in the third year, the lysimeter was instrumented with porous cup samplers and the same experimental design repeated on a smaller scale.

A convection-dispersion (CDE) model was applied to the lysimeter data. This was successful, provided that the surface soil and assumed Dirac delta solute input were not included in the calibration. Layering within the profile appeared to have little effect on solute transport. The transport porosity was revealed to be two-thirds of the water-filled porosity, thus a substantial part of the water-filled porosity did not transport solute. The CDE modelling of the field data was not particularly

successful, probably due to the spatially variable nature of solute transport and water application.

The Aggregated Mixing Zone (AMZ) model was also used. This model subdivided the transport porosity into convective and dispersive components, and also allowed for non-interacting flow paths. Although the AMZ model was conceptually appealing, parameterisation of the model was found to lack discrimination. Little further understanding of solute transport was gained from this model.

Textural differences in the soil seem to be overwhelmed by both small-scale heterogeneity of water application and solute movement in the soil, especially near to the surface. It was apparent that processes occurring in the surface soil require much more attention than they have been afforded in the past.

Both process-based modelling and field experimentation will increase our understanding of solute transport. It also seems that an increased effort in improving measurement techniques will be advantageous.

ACKNOWLEDGEMENTS

Funding for the work done in this thesis was provided by two organisations that, as a result of recent restructuring, no longer exist. They were the Ministry of Works and Development and the Department of Scientific and Industrial Research.

Thanks are due to Professor Bob White, now at School of Agriculture and Forestry at the University of Melbourne, who was chief supervisor for much of the time. He initiated the work and sought the initial funding.

Dr Dave Scotter, of the Department of Soil Science, provided background guidance and thoughtful discussion throughout the thesis, and later became chief supervisor. Thanks for this as well as the discussions of choice tramping spots in the Ruahines.

Dr Brent Clothier (Environmental Physics Group, HortResearch) found himself co-opted informally, and then formally onto the supervision team. During this study he gave freely of his time and provided much zestful argument, as well as friendship. Brent also was closely involved in the final writing of the thesis. Without his inspiration, encouragement and guidance the thesis probably would not have been completed within the deadline. He deserves, and has, my great appreciation.

The last appointment to the supervisory team was Dr Paul Austin, then of the Department of Production Technology at Massey University, but now at Cambridge Control, Cambridge, United Kingdom. Paul encouraged a line of research that probably would otherwise have been ignored and, as well as his modelling skills, brought a different perspective to many discussions. I hope he appreciated the ensuing debate.

At various times the following people assisted in the field work.

Katy Grainger and Hugh Forlong helped instrument the field. Hugh also carried on with the experimental work while I was ill in 1988.

Most of the students in the Department of Soil Science in 1989 helped spread fertiliser on the plot.

Malcolm Boag, Dave Scotter, and Alistair Pickens tried to help me get the irrigation system started in 1989, fought over who would get to wear the Gortex raincoat, and provided solace when it wasn't needed.

Ross Wallace and especially Ian Furkert helped with those jobs that just couldn't be done by one person, such as mowing the 0.35 ha plot with standard lawnmowers.

John Julian deserves special mention. He helped organise equipment, coaxed the irrigation pump, did all sorts of jobs that made the field work possible, and terrified me with his cross-country driving.

Thanks to all these people and to those whose, although not included formally here, efforts are nevertheless appreciated.

Thanks to Dave Barker for the final proof reading of the thesis. This was much appreciated.

Jacque Rowarth, Prue Williams, Peter Kemp, and Robyn Simcock all proved to be wonderful friends during this study. Thanks also to the members of the Manawatu Tramping and Skiing Club with whom I spent too many sanity-preserving days, both enjoyable and miserable, in New Zealand's wonderful forests, rivers, and mountains.

TABLE OF CONTENTS

ABSTRACT	ii
ACKNOWLEDGMENTS	iv
TABLE OF CONTENTS	vi
LIST OF FIGURES	x
LIST OF TABLES	xiii
LIST OF SYMBOLS	xv

Chapter One INTRODUCTION

1.1 INTRODUCTION	1
1.2 A HISTORICAL PERSPECTIVE OF SOLUTE TRANSPORT	3
1.3 ISSUES OF SOLUTE TRANSPORT ADDRESSED IN THIS THESIS .	7
1.4 EXPERIMENTAL APPROACH ADOPTED IN THIS THESIS	9
1.5 SUMMARY	11

Chapter Two SOIL, SITE AND EXPERIMENTAL METHODS

2.1 SITE AND SOIL	12
2.1.1 Soil description	12
2.1.2 Lysimeter description	14
2.2 INSTRUMENTATION	15
2.2.1 Field plot layout	15
2.2.2 Neutron probe measurements	15
2.2.3 Soil solution sampling	19
<i>Construction</i>	19
<i>Installation</i>	19
<i>Sample collection</i>	20
2.2.4 Time domain reflectometry	20
2.2.5 Meterological measurements	21
<i>Evapotranspiration calculation</i>	22
2.2.6 Irrigation system	23
2.3 1988 LEACHING EXPERIMENT	23
2.4 1989 LEACHING EXPERIMENT	29

2.5	1990 LEACHING EXPERIMENT	31
2.6	CHEMICAL ANALYSES	32
2.6.1	Soil solution samples	33
	<i>Chloride</i>	33
	<i>Bromide</i>	34
2.6.2	Soil cores	34
	<i>Chloride</i>	35
2.6.3	Herbage	35

Chapter Three RESULTS AND DISCUSSION

3.1	1988 DATA	36
3.1.1	Water Balance	36
3.1.2	Porous Cup Samples and Lysimeter Outflow	41
	<i>Characteristic Sites</i>	41
	<i>Bulked Data</i>	43
	<i>Lysimeter Data</i>	44
3.1.3	Soil Cores	46
3.1.4	Chloride Mass Balance	46
3.2	1989 DATA	48
3.1.1	Water Balance	48
3.2.2	Porous Cup Samples and Lysimeter Outflow	49
	<i>Characteristic Sites</i>	49
	<i>Bulked Data</i>	51
	<i>Lysimeter Data</i>	52
3.2.3	Soil Cores	52
3.2.4	Chloride Mass Balance	54
3.3	1990 DATA	55
3.3.1	Water Balance	55
3.3.2	Porous Cup and Lysimeter Data	56
3.3.3	Bromide Mass Balance	56
3.4	Comparison of Cup and Core Samples	57
3.5	Computing the Field Average Solute Flux	62
3.6	Spatial Variability	67
3.7	Comparison of Lysimeter Drainage in 1988 and 1990	74
3.8	Summary	75

Chapter Four
CONVECTIVE-DISPERSIVE MODELLING OF SOLUTE TRANSPORT

4.1	INTRODUCTION	77
4.2	THEORY	77
	4.2.1 The Convection-Dispersion Equation and its Application to Field-Scale Transport	78
	4.2.2 The Transfer Function Model	81
4.3	METHODOLOGY	85
4.4	APPLICATION OF THE CDE TO THE 1990 LYSIMETER DATA ..	86
4.5	APPLICATION OF THE CDE TO THE 1988 FIELD DATA	94
4.6	CONCLUSIONS	95

Chapter Five
THE AGGREGATED MIXING ZONE MODEL

5.1	INTRODUCTION	97
5.2	THE AMZ MODEL	98
	5.2.1 Solute transport through a single tank	98
	5.2.2 Solute transport through a network of tanks	102
	5.2.3 Model structure identification and parameterisation	105
	5.2.4 Prediction of solute transport through a network of tanks	110
5.3	AMZ MODEL PARAMETERISATION	112
5.4	SIMULATING THE EFFECT OF VARYING MODEL STRUCTURE AND PARAMETERS	113
	5.4.1 Effect of varying V_c and V_m in a single tank	114
	5.4.2 Effect of varying n , the number of tanks	116
	5.4.3 Effect of varying x , the number of pathways	118
5.5	PRELIMINARY INVESTIGATION OF THE AMZ MODEL	120
	5.5.1 ARMA equation structure differentiation	122
	5.5.2 Application of the AMZ model to the 1990 lysimeter data	124
	5.5.3 Application of the AMZ model to the Aggregated 1988 field data	128
	5.5.4 ARMA Equation Factorisability	131
5.6	CONCLUSION	137

Chapter Six
DISCUSSION AND CONCLUSIONS

6.1 INTRODUCTION	139
6.2 INFORMATION GAINED EMPIRICALLY	140
6.3 UNDERSTANDING GAINED FROM THE CDE MODEL	141
6.4 UNDERSTANDING GAINED FROM THE AMZ MODEL	143
6.5 EMPIRICISM AND MODELLING: IMPLICATIONS FOR USERS .	144
6.6 EMPIRICISM AND MODELLING: IMPLICATIONS FOR RESEARCHERS	146
6.7 SUMMARY	148

Appendix A
DERIVATION OF EQUATION (5.3)

.....	151
-------	-----

Appendix B
DERIVATION OF EQUATION (5.5)

.....	153
-------	-----

Appendix C
FACTORISATION OF THE ARMA EQUATION

.....	155
-------	-----

REFERENCES

.....	159
-------	-----

List of Figures

Figure 1.1	A philosophical framework for the understanding of solute transport	5
Figure 2.1	Field plot layout	17
Figure 2.2	Scatter plot of θ measured by gravimetric sampling against that from equation (2.1)	18
Figure 3.1	Cumulative irrigation input to each site ^{and} the lysimeter. Day 0 was 27 April 1988	37
Figure 3.2	Water balance for the 1988 experiment showing evapotranspiration, irrigation, and rainfall, as well as measured and estimated drainage	39
Figure 3.3	Measured and estimated drainage from the lysimeter in 1988 with enforced equality on day 85	40
Figure 3.4	Porous cup concentrations at sites 12, 14, 16, and 19, in 1988	42
Figure 3.5	Porous cup concentrations for all sites and depths in 1988	44
Figure 3.6	Solute concentration and se in the 1988 soil cores. Concentration is expressed per volume of soil solution	45
Figure 3.7	Water balance for the 1989 experiment, showing evapotranspiration and rainfall, as well as measured and estimated drainage for the lysimeter. Day 0 was 21 June 1989	49
Figure 3.8	Porous cup concentrations at sites 12, 14, 16, and 19 in 1989	50
Figure 3.9	Porous cup concentrations for all sites and depths in 1989	51
Figure 3.10	Soil solution concentration in the 1989 soil cores	53
Figure 3.11	Water balance for the 1990 experiment showing evapotranspiration, rainfall, irrigation, as well as measured and estimated drainage. Day 0 was 23 July 1990	55
Figure 3.12	Porous cup and outflow concentrations in the 1990 lysimeter experiment	56
Figure 3.13	Comparison of solute concentration from soil core and porous cup samples. Note the changes of scale in the vertical axis	60

Figure 3.14 Comparison of field average solute flux as given by equations (3.6) and (3.11)	66
Figure 3.15 Field-average BTC's derived by calculation from parameters of individual data and from fitting to the bulked data	72
Figure 3.16 Solute BTC at 1000 mm for 1988 determined from the lysimeter outflow as well as the porous cup samples	73
Figure 3.17 Solute BTC from the lysimeter in 1988 and 1990	74
Figure 4.1 Data from the 1990 lysimeter and, a) a CDE calibrated to the 250 mm data and predicted at 550 mm, 760 mm, and 1000 mm, and b) a CDE calibrated to each depth	89
Figure 4.2 1990 lysimeter data and a CDE calibrated with the 250 mm data as the input and the 550 mm data as the output, as well as the predictions to 760 mm and 1000 mm	93
Figure 5.1 A continuously-stirred tank, showing the convective volume, V_c , and the mixed volume, V_m	99
Figure 5.2 A diagrammatic representation of the AMZ for two solute transport pathways, one pathway with two tanks, the other with one tank	103
Figure 5.3 Flow chart showing the AMZ modelling process	111
Figure 5.4 The effect of varying V_c and V_m on output solute concentration	115
Figure 5.5 The effect of varying n on output solute	116
Figure 5.6 The effect of varying both n and depth on output solute concentration	117
Figure 5.7 The effect of more the one solute transport pathway on output solute concentration	119
Figure 5.8 The effect of changing the ARMA equation structure on the calibration mse	123
Figure 5.9 AMZ model calibration between 250 mm and 550 mm for the 1990 lysimeter data	126

Figure 5.10	AMZ model predictions for solute concentration at, (a) 760 mm, and, (b) 1000 mm for the 1990 lysimeter data	127
Figure 5.11	Calibrated ARMA equation and AMZ model output for the aggregated field data. The error bars show the ± 1 se for the data	130
Figure 5.12	AMZ model predictions for the aggregated field data at, (a) 760 mm, and, (b) 1000 mm	131
Figure 5.13	ARMA equation and AMZ model calibration for solute transport between 250 mm and 550 mm at site 10	132
Figure 6.1	A philosophical framework for the understanding of solute transport modified by the experience of this thesis	149

List of Tables

Table 2.1	Soil description (Clothier, 1977)	13
Table 2.2	Soil bulk density (ρ_b) standard deviation (sd), number of samples (N) for the three layers of the Manawatu fine sandy loam	14
Table 2.3	Interface depths, and depth of the deepest sampler	16
Table 2.4	1988 soil solution sampling dates, and average cumulative drainage on that day	28
Table 2.5	1988 soil coring dates. N is the number of samples at each depth	27
Table 2.6	1989 soil solution sampling dates	30
Table 2.7	1989 soil coring dates. N is the number of samples at each depth	31
Table 3.1	Chloride mass balance for the 1988 experiment, showing the amount of solute present in the soil at the beginning and end of the experiment as well as the solute in drainage water, irrigation water and in the fertiliser	48
Table 3.2	Bromide mass balances, calculated from equation (3.2), as well as bromide in the drainage water	57
Table 3.3	Statistically significant correlation coefficients between c and I . Here ρ_s is the Spearman correlation	65
Table 3.4	Lognormal distribution parameters for the 1988 BTC's calculated by either fitting equation (3.13) to the individual site data and then averaging or by fitting to the bulked data	71
Table 3.5	Expectation and variance, calculated from equations (3.14) and (3.15), of the solute BTC's from either the individual site or the bulked data	71
Table 3.6	Mean, standard deviation, and median for the BTC's from the lysimeter outflow in 1988 and 1990	74

Table 4.1	Coefficients of the CDE fitted to the 1990 lysimeter data with a Dirac delta function at the soil surface as the input. Dispersivity is also given	87
Table 4.2	Calibrated CDE parameters of the Fickian transfer function, and the dispersivity. These result from using the data measured at 250 mm in the lysimeter as the input function	91
Table 4.3	CDE parameters fitted to the 1988 field data with either a Dirac delta function at the soil surface or the data measured at 250 mm as the input function	94
Table 5.1	Example ARMA equations and associated AMZ models	121
Table 5.2	Site 12 ARMA and AMZ model structures	124
Table 5.3	ARMA and AMZ parameter values for solute transport between 250 mm and 550 mm in the lysimeter	125
Table 5.4	ARMA equation and AMZ parameter values for solute transport between 250 mm and 550 mm in the aggregated field data	129
Table 5.5	Site 10 ARMA equation and AMZ model structures	133
Table 5.6	The calibrated ARMA equation parameters and equivalent ARMA equation parameters back-calculated from the AMZ model for site 10 between 250 mm and 550 mm. (* parameters used to calculate the AMZ model)	136

List of Symbols

a_i	parameter in A	-
b_i	parameter in B	-
c	soil solution concentration	$M L^{-3}$
c'	flux concentration	$M L^{-3}$
c'	resident soil solution concentration	$M L^{-3}$
c^ϕ	field-scale soil solution concentration	$M L^{-3}$
c_i	input solute concentration	$M L^{-3}$
c_o	output solute concentration	$M L^{-3}$
c_p	concentration in rainfall	$M L^{-3}$
c_r	concentration in irrigation	$M L^{-3}$
e	error, deviation of model from data	-
f	solute travel-time probability density function	T^{-1}
f	defined by equation (A.8)	-
g	solute life-time probability density function	T^{-1}
g	defined by equation (A.9)	-
i	dummy variable	-
j	number of intervals of cumulative drainage	-
j	dummy variable	-
k_i	AMZ model parameter, defined by (5.14)	-
l	dummy variable	-
n	dummy variable (Appendix B)	-
n_a	number of a_i parameters in A	-
n_b	number of b_i parameters in B	-
n_c	number of c_i parameters in C	-
n_d	number of d_i parameters in D	-
n_f	number of f_i parameters in F	-
n_i^z	number of tanks in i^{th} series at depth z	-
n_k	number of delays on the ARMA input	-
q^{-1}	delay operator	-
s	slope of the saturated water vapour curve	$M L^{-1} T^{-2}$
s	Laplace variable (Ch. 5)	-

t	time	T
v	pore-water velocity	L T ⁻¹
x	number of pathways	-
x_i	proportion of water passing through i^{th} path	-
z	depth or calibration depth	L
A	cross-sectional area	L ²
A	ARMA equation polynomial	-
B	ARMA equation polynomial	-
C	ARMA equation polynomial	-
C	Laplace transform of c	-
C_i	Laplace transform of c_i	-
C_o	Laplace transform of c_o	-
C_r	count ratio	-
D	dispersion coefficient	L ² T ⁻¹
D	ARMA equation polynomial (Ch. 5)	-
E	evapotranspiration rate	L ³ L ⁻² T ⁻¹
F	ARMA equation polynomial	-
F	defined by equation (A.2)	-
H	total solute uptake by herbage	M L ⁻²
I	cumulative drainage density	L ³ L ⁻²
\bar{I}	average drainage density	L
I^ϕ	field-average drainage	L ³ L ⁻²
J^ϕ	field-average solute flux	M L ⁻² T ⁻¹
J_w	water flux	L T ⁻¹
L	calibration depth	L
M	amount of applied solute	M L ⁻²
N	number of samples	-
P	rainfall	L ³ L ⁻²
Q	water flow rate	L ³ T ⁻¹
Q	cumulative drainage	L ³
Q_{in}	solute mass entering soil volume	M
Q_{out}	solute mass leaving soil volume	M
R	irrigation	L ³ L ⁻²

R_n	net radiation per unit area and time	$M T^{-3}$
V_c	convective volume	L^3
V_m	mixed volume	L^3
V_t	total volume	L^3
Z	prediction depth	L
α_i	AMZ model parameter, defined by (5.12)	-
β_i	AMZ model parameter, defined by (5.13)	-
γ	psychometric constant	$M L^{-1} T^{-2}$
θ	volumetric water content	$L^3 L^{-3}$
$\hat{\theta}$	estimated volumetric water content	$L^3 L^{-3}$
θ_{st}	transport porosity	$L^3 L^{-3}$
θ_{im}	porosity inactive in solute transport	$L^3 L^{-3}$
θ_{TDR}	θ measured with a TDR	$L^3 L^{-3}$
λ	dispersivity	L
λ	latent heat of vaporisation of water (Ch. 2)	$L^{-2} T^{-2}$
μ	mean of the lognormal distribution	-
μ_{field}	field average mean of lognormal distribution	-
ρ_b	bulk density	$M L^{-3}$
ρ_s	Spearman correlation coefficient	-
ρ_w	density of water	$M L^{-3}$
σ	standard deviation of the lognormal distribution	-
σ_{field}	field average of the lognormal distribution	-
τ	input time	T
\mathcal{L}	Laplace operator	
E	expectation	
E_f	expectation at field scale	
E_l	expectation at local scale	
E_{field}	expectation of field-average BTC	
Var	variance	
Var_f	variance at field scale	
Var_l	variance at local scale	
Var_{field}	variance of field-average BTC	
Cov	covariance	