



THE UNIVERSITY  
*of* ADELAIDE

---

Assessing Natural and Management-Induced Patterns  
of Herbicide Sorption and Risks in Catchments:  
*A Soil Landscape Modeling Approach*

---

A thesis submitted to the University of Adelaide in fulfillment of the requirements  
for the degree of Doctor of Philosophy in Science

**BENG P. UMALI**

*M.Sc. Forestry, University of the Philippines Los Baños*

Ecology, Evolutionary Biology and Landscape Science  
School of Earth and Environmental Sciences

March 2012



## Abstract

*The overall aim of this thesis was to study the natural and landscape-induced patterns of herbicide sorption and risks of leaching and off-site transport of herbicides in an intensively managed orchard system. The questions for this thesis were: a) How can contour-derived digital elevation models be enhanced? b) To what extent do topographic and management factors influence the distribution of soil properties in an apple orchard? c) How do landscape topography, soil properties and land management factors influence the spatial distribution of diuron sorption affinity? and d) How is the fate of diuron influenced by the spatial variability of soil and key fate properties?*

*The objectives of this thesis were: a) to determine whether a 'smoothing' algorithm can enhance the accuracy of a contour-derived digital elevation model; b) to evaluate the role of topography and management practises in predicting the distribution of soil properties using a soil-landscape modeling approach; c) to evaluate the effects of topography, soil properties and management practises on the sorption affinity of diuron; and d) to assess the integrated effect of topography, management practises and herbicide sorption on the leaching potential of diuron in a spatially variable landscape using the Leaching Estimation and Chemistry Model (LEACHM) and surface runoff using the Organization for Economic Cooperation and Development (OECD) model.*

*A study site in the Mount Lofty Ranges, South Australia, was selected for its wide variation in landscape and soil properties under intensive horticultural management. The site was a section of an apple orchard with a strong texture contrast soil and landform with a relief difference of 50 m. The accuracy of digital elevation models (DEMs) of the site was first evaluated. Then the relationship between terrain*

*parameters and critical soil properties that were easily determined in the field (e.g. soil colour and texture) was determined. A strong relationship was found and therefore the experiment was expanded to take into account the effects of management and terrain on soil properties that influence pesticide sorption, such as total organic carbon, soil pH, electrical conductivity, clay content, and soil texture. Sorption of the herbicide diuron was determined on the soil through traditional laboratory and chemometric analyses using mid-infrared (MIR) spectroscopy. A strong correlation was found between diuron sorption coefficient values determined by traditional laboratory methods and those predicted using MIR spectroscopy ( $R^2 = 0.79$ ).*

*Then, the determination of the effects of terrain properties and management practises on diuron sorption distribution was evaluated within the context of soil-landscape analysis and geostatistical mapping. Soil properties varied significantly between alley and tree line regions and among different establishment ages of the orchard trees. Unique spatial patterns for soil properties, particularly total organic carbon (TOC), occurred within zones of the orchard. The variability in spatial distribution of the soil properties was reflected in the amount of diuron sorbed to the different soils. In the tree-line, where the soil was kept bare, diuron sorption affinity was significantly 16% lower than in the alley, where sod strips protected the soil surface all year round.*

*Finally, leaching of diuron was estimated using LEACHM and the potential for surface runoff of diuron was determined using the OECD model. Management practises, the level of TOC and slope were found to influence leaching and runoff potential of diuron.*

*The findings imply that, for intensively managed horticultural operations on complex landscapes, the influence of terrain on the distribution of soil properties and*

*consequently on diuron sorption affinity was masked by management factors. Assessments of sorption distribution and, therefore, the environmental fate of pesticides must include stratification strategies based on management factors. The leaching estimation also suggests variable risk of diuron for mobility based on management and TOC. Therefore, a differential herbicide and pesticide application or management regime might need to be observed to minimise off-site impact of pesticides.*

## **Acknowledgement**

Thanks to all my supervisors especially to Rai and Bertram: I appreciate the guidance you have extended to me and for your patience. The support you have given me far exceeded my expectations. Thanks also to Danni who patiently guided me in experiments, field work and writing up; David for your insights in Pedology and for encouraging me do more; and to to John, who sat countless hours with me in front of the computer, so that I learn the ropes of LEACHM. The knowledge I gained during the last four years will be treasured and propagated.

I appreciate the lessons shared, camaraderie and friendship from all the SIGers: Greg, Ken, Ramesh, Adam, Bart, Dave, Joel, Tori, Erica, Leo, Davina, Sirhey, Chris; and the Soils Group people: Ana, Jia, Margaret, Nang, Ashlea, Sarah, Geert, Sola, Raj, Hasnuri, Tra, Narges and Alla. To Jose and Max, thanks for helping me out in the field. Thanks also to Nigel Fleming and Mark Agnew of the South Australian Research and Development Institute (SARDI) for lending me the EPOCH 10 RTK GPS system and assisting me in all of my survey campaigns. To Peta Jacobsen for giving me advise in setting up those delicate capacitance moisture probes. To Dr. Mohsen Forouzangohar and Sean Forester for teaching me the rudiments of MIR-PLS. To Dr. Ron Smernic for your guidance in writing and for the pep talks. To Dr. Margaret Cargill for the valuable comments on my proposal and some of my initial manuscripts. To Dr. Megan Lewis, our SIG head, who never tire providing the much needed moral support not only to her advisees but all SIG students. I was also fortunate to be guided by two highly diligent Postgrad Coordinators: Drs. Cam Grant (AFW) and John Jennings (EES).

Thanks to Nirajala Seimon and all the wonderful people at the International Student Centre.

My deepest gratitude goes to the Australian Centre for International Agricultural Research for providing me the John Allwright Fellowship and to Cavite State University for granting me leave of study.

To all who helped me in the laboratory, thanks for making my life easy: Colin Rivers (UniAdelaide), Lester Smith, Jill Cozens, and Jenny Anderson (CSIRO-Land and Water). And the EES people: Marie, Debbie, Sue, Gary.

To all my Pinoy friends in Adelaide, thanks for being there for me and my family- never did we feel that Adelaide is a foreign place.

Thanks to my parents, Dr. Cesar G. Umali and Realtor/Councilor Nona P. Umali, and to all my siblings for your prayers and encouragement.

To my loving wife **Mariane**, thank you – you not only stood by me, you also joined me each step of the way with delight and much more passion... and to my sweet daughter **Bea**, you've taught me things more than I imagined....

...and most importantly

***To our Loving God, my redeemer and source of strength...***

## Table of Contents

<b>ABSTRACT</b>	<b>I</b>
<b>I. INTRODUCTION</b>	<b>1</b>
1. RESEARCH BACKGROUND	1
2. RESEARCH OBJECTIVES	2
3. THESIS STRUCTURE	3
<b>II. LITERATURE OVERVIEW</b>	<b>5</b>
1. PESTICIDES AND THE MODERN AGRICULTURAL PRODUCTION	5
2. THREAT OF PESTICIDES TO THE ENVIRONMENT	6
3. MATHEMATICAL MODELING OF PESTICIDE FATE	8
4. SOIL-LANDSCAPE ANALYSIS IN ASSESSING PESTICIDE FATE	10
<b>III. QUALITY ASSESSMENT OF A TOPOGRAPHICALLY DERIVED HIGH-RESOLUTION DIGITAL ELEVATION MODEL OF A SOUTH AUSTRALIAN SLOPING LANDSCAPE</b>	<b>19</b>
1. INTRODUCTION	20
2. METHODOLOGY	23
2.1. STUDY SITE	23
2.2. DIGITAL ELEVATION MODELS	23
2.3. FIELD EVALUATION DATA	24
2.4. ANALYSIS	25
3. RESULTS	26
3.1. INTERPOLATION AND SMOOTHING OF DEM	26
3.2. VALIDATION OF SUBCATCHMENT ELEVATION	28
3.3. QUALITY OF RTK DEM	29
3.4. ASSESSMENT OF TOPOGRAPHICALLY DERIVED DEM	29
4. DISCUSSION	30
5. CONCLUSION	32
<b>IV. SPATIAL HETEROGENEITY OF SOIL PROPERTIES TO PREDICT PESTICIDE MOVEMENT</b>	<b>51</b>
1. INTRODUCTION	52
2. METHODOLOGY	54
2.1. STUDY SITE	54
2.2. SOIL DATA COLLECTION	54
2.3. GENERATION OF DEM AND CALCULATION OF TOPOGRAPHIC VARIABLES	55
2.4. IDENTIFICATION OF LAND SURFACE ZONES	56
2.5. STATISTICAL ANALYSIS	56
3. RESULTS AND DISCUSSION	57
3.1. SOIL COLOUR AND TEXTURE IN THE APPLE ORCHARD	57
3.2. TERRAIN ATTRIBUTES AND SOIL PROPERTIES	58
4. CONCLUSION	60
<b>V. EFFECT OF TERRAIN AND MANAGEMENT ON THE SPATIAL VARIABILITY OF SOIL PROPERTIES IN AN APPLE ORCHARD</b>	<b>69</b>
1. INTRODUCTION	70
2. MATERIALS AND METHODS	73



2.1.	SITE DESCRIPTION AND GENERAL METHODOLOGICAL APPROACH	73
2.2.	DEM AND DTM GENERATION	73
2.3.	APPLE ORCHARD MANAGEMENT	74
2.4.	SOIL SAMPLING AND ANALYSIS	75
2.5.	STATISTICAL ANALYSIS	76
2.6.	REGRESSION AND GEOSTATISTICAL PREDICTION OF SOIL PROPERTY DISTRIBUTION	77
<b>3.</b>	<b>RESULTS</b>	<b>79</b>
3.1.	VARIABILITY OF SOIL PROPERTIES	79
3.2.	UNIVARIATE SPATIAL DEPENDENCE ANALYSIS OF SOIL PROPERTIES	79
3.3.	SOIL LANDSCAPE ANALYSIS AND MODELLING	80
3.4.	PREDICTION OF SOIL PROPERTIES	81
<b>4.</b>	<b>DISCUSSION</b>	<b>82</b>
<b>5.</b>	<b>CONCLUSION AND RECOMMENDATION</b>	<b>85</b>
<b>VI.</b>	<b>SPATIAL DISTRIBUTION OF DIURON SORPTION AFFINITY AS AFFECTED BY SOIL, TERRAIN AND MANAGEMENT PRACTISES IN AN INTENSIVELY MANAGED APPLE ORCHARD</b>	<b>104</b>
<b>1.</b>	<b>INTRODUCTION</b>	<b>105</b>
<b>2.</b>	<b>METHODOLOGY</b>	<b>107</b>
2.1.	STUDY SITE, SOIL SAMPLING AND TERRAIN PARAMETERIZATION	107
2.2.	DIURON SORPTION DETERMINATION BY MID-INFRARED SPECTROSCOPY	109
2.3.	STATISTICS AND MODELING SPATIAL DISTRIBUTION OF DIURON K <sub>d</sub> VALUES	112
<b>3.</b>	<b>RESULTS AND DISCUSSION</b>	<b>113</b>
3.1	PREDICTION OF DIURON K <sub>d</sub> AFFINITY USING MIR-PLS MODEL	113
3.2	RELATIONSHIP OF DIURON K <sub>d</sub> WITH SOIL PROPERTIES AND TERRAIN PARAMETERS	114
3.3	SORPTION OF DIURON IS AFFECTED BY DIFFERENTIAL MANAGEMENT BETWEEN ALLEY AND TREE LINE	117
<b>4.</b>	<b>CONCLUSION</b>	<b>119</b>
<b>VII.</b>	<b>FIELD-SCALE VARIABILITY OF SIMULATED DIURON LEACHING AND SURFACE RUNOFF IN AN INTENSIVELY MANAGED APPLE ORCHARD</b>	<b>136</b>
<b>1.</b>	<b>INTRODUCTION</b>	<b>137</b>
<b>2.</b>	<b>METHODOLOGY</b>	<b>138</b>
2.1	STUDY AREA AND DIURON	138
2.2	DESCRIPTION OF LEACHP	140
2.3	DESCRIPTION OF THE MODELING SCENARIO	142
2.4.	LEACHM OUTPUT SIMULATION PARAMETERS: FLUX, RETENTION AND LOADING	145
2.5.	PESTICIDE RUNOFF SIMULATION USING THE OECD MODEL	146
<b>3.</b>	<b>RESULTS AND DISCUSSION</b>	<b>147</b>
3.1.	EFFECTS OF SOIL WATER CONTENT AND IRRIGATION ON SIMULATED FLUX AND RETENTION	147
3.2.	EFFECT OF CLAY AND ORGANIC CARBON CONTENTS ON THE SIMULATED FLUX AND RETENTION	148
3.3.	EFFECT OF CROPPING SYSTEM/CROP COVER ON THE SIMULATED FLUX AND RETENTION	149
3.4.	EFFECT OF SLOPE ON SIMULATED PESTICIDE RUNOFF	149
3.5.	SEASONAL VARIABILITY OF SIMULATED FLUX, RETENTION AND PESTICIDE RUNOFF OF DIURON	150
3.6.	EFFECT OF MANAGEMENT ON SIMULATED FLUX, RETENTION AND LOADING	151
<b>4.</b>	<b>CONCLUSION</b>	<b>152</b>
<b>VIII.</b>	<b>OVERALL SUMMARY, CONCLUSION AND RECOMMENDATIONS</b>	<b>170</b>



## List of Tables

Table II.a.	Examples of simulation models used to predict pesticide behaviour classified according to purpose (Wagenet and Rao, 1990).	9
Table III.a.	Digital elevation model datasets used in this study, all using 5 m pixel.	37
Table III.b.	Terrain parameters calculated in this study.	38
Table III.c.	Summary statistics of spot heights (m) derived from different elevation sources.	38
Table III.d.	Quality of DEM derived from interpolated real-time kinematic GPS survey for the subarea.	39
Table IV.a.	Terrain attributes calculated in the study (Farenhorst et al., 2008; Florinsky et al., 2002; Gallant and Wilson, 2000).	63
Table IV.b.	G-test of independence between terrain attributes and soil colour (value)	63
Table IV.c.	G-test of independence between terrain attributes and texture	64
Table V.a.	Terrain parameters calculated in this study.	92
Table V.b.	Summary statistics of properties for soils sampled in alleys and in tree lines.	93
Table V.c.	Summary table of model parameters for soils properties using stepwise linear regression with Akaike Information Criterion.	94
Table V.d.	Results of the jack-knife validation of the three prediction models	95
Table VI.a.	Summary statistics of soil properties and diuron $K_d$ determined for soils from alley and tree line.	125
Table VI.b.	Correlation matrix of diuron sorption affinity ( $K_d$ ), soil properties and terrain parameters for alley (in bold) and tree-line (in bold-italics).	126
Table VI.c.	Soil landscape models for diuron $K_d$ using Partial least squares (PLS) regression.	127
Table VII.a.	Summary statistics of selected soil, pesticide and terrain properties in the alley and tree-line regions in the apple orchard used in the LEACHP simulation.	157
Table VII.b.	Total monthly rainfall for the designated month considered in the simulation (BOM, 2011).	157
Table VII.c.	Summary statistics of simulated Retention and Flux for alley and tree line (in brackets) (n=100) during three simulation periods.	158
Table VII.d.	Mean comparison of simulated Flux, Retention and Loading among zones for July 2006; TOC means of zones were put for reference (Umali et al., 2012b).	159

## List of Figures

Figure III.a.	Location of the study site (Red circles mark broken and overlapping contour lines. Aerial photograph taken 26 December 2009 is from <a href="http://www.nearmap.com">www.nearmap.com</a> available under Creative Commons Attribution Share Alike license).	40
Figure III.b.	DEM of the site (a - raw10K, b - smooth10K, c - raw50K, d - smooth50K).	41
Figure III.c.	Histograms of contour-derived DEM from (a) 1:10,000 and (b) 1:50,000 topographic maps.	42
Figure III.d.	Profile curvature of unsmooth (a) and smooth (b) DEM derived from 1:10,000 contour data (pixel size = 5 m).	43
Figure III.e.	Survey points and digital elevation model from real-time kinematic global positioning system (RTK-GPS) survey.	44
Figure III.f.	Residuals of the (a) elevation, (b) slope, (c) plan curvature, and (d) profile curvature for each DEM against rtk DEM.	46
Figure III.g.	Scatterplots and correlation coefficient values of digital elevation models (a) elevation, (b) Slope, (c) plan curvature, and d) profile curvature) from different sources.	47
Figure IV.a.	Location of study site and sampling points (red dots).	65
Figure IV.b.	Landsurface zones	66
Figure V.a.	Location map of the study site (Each × represents a sampling location of two samples, one in the alley and one in the tree line).	96
Figure V.b.	Digital terrain models generated from topographic and drainage maps of the study site (contour lines in gray are from 490 m at the top right to 540 m at the bottom left). PlanC – plan curvature; ProfC – profile curvature; TanC – tangential curvature; RSP – relative stream power; SCA – specific catchment area, $m^2m^{-1}$ ; STCI – sediment transport capacity index; WI - wetness index).	97
Figure V.c.	Variograms of total organic carbon (%) in the alley (a) and tree line (b), $pH_w$ in the alley (c) and tree line (d), log normal electrical conductivity in the alley (e) and tree line (f), per cent clay in the alley (g) and tree line (h), and per cent coarse fraction in the alley (i) and tree line (j).	98
Figure V.d.	Pearson correlation coefficients of soil properties and terrain parameters.	99
Figure V.e.	Predicted map of total organic carbon (a), and coarse fraction (b), of the study site using ordinary kriging (both properties are in %; hatched area is the tree line, the rest is alley; contour lines at 5 m interval from 490 m in the top right to 540 m in the bottom left).	100
Figure VI.a.	Partial Least Squares (PLS) loading weights of the first two factors used in the regression model.	128
Figure VI.b.	Relationship between diuron $K_d$ values predicted using MIR-PLS and those determined on the subset (n=46; 4 outliers were	

	removed) of samples using the traditional batch sorption techniques (dotted line is the 1 is to 1 line; SECV is standard error of the cross-validation). MIR-PLS – mid-infrared partial least squares technique	129
Figure VI.c.	Loading weights of the first factor for alley and tree-line of the Partial Least Squares (PLS) regression using soil and terrain variables as predictors.	130
Figure VI.d.	Interpolated map of diuron $K_d$ ( $\text{kg L}^{-1}$ ) for the study site.	131
Figure VI.e.	Means of diuron $K_d$ (lower data, $\text{L kg}^{-1}$ ) and total organic carbon (upper data, %) in the different management zones and sampling locations.	132
Figure VII.a.	An orthophotograph of the study site showing the management zones in capital letters.	160

## **Declaration**

This work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution to me and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

I give consent to this copy of my thesis, when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968.

The author acknowledges that copyright of published works contained within this thesis (as listed in the next page) resides with the copyright holder(s) of those works.

I also give permission for the digital version of my thesis to be made available on the web, via the University's digital research repository, the Library catalogue, the Australasian Digital Theses Program (ADTP) and also through web search engines, unless permission has been granted by the University to restrict access for a period of time.

BENG P. UMALI

## **Publications and Conference Papers and Presentations arising from this thesis**

### Journal Article (published, accepted or in preparation)

Umali, B.P., Oliver, D.P., Forrester, S.T., Chittleborough, D.J., Hutson, J.L., Kookana, R.S. and Ostendorf, B.F. 2012. The effect of terrain and management on the spatial variability of soil properties in an apple orchard. *Catena*. 93: 38-48.

Umali, B.P., Oliver, D.P., Ostendorf, B., Forrester, S., Chittleborough, D.J., Hutson, J.L. and Kookana, R.S. 2012. Spatial distribution of diuron sorption affinity as affected by soil, terrain and management practises in an intensively managed apple orchard. *J. Haz. Mat*, 217-218: 398-405.

Umali, B.P., Clarke, K., Ostendorf, B. Quality Assessment of a Topographically Derived High-Resolution Digital Elevation Model of a South Australian Sloping Landscape. Submitted to the *Journal of Spatial Science*.

Umali, B.P., Hutson, J.L., Oliver, D.P., Ostendorf, B., and Kookana, R.S. Field-scale variability of simulated diuron leaching and surface runoff in an intensively managed apple orchard. Manuscript in preparation.

### Refereed Conference Paper (with presentation)

Umali, B.P., Kookana, R.S., Oliver, D.P., Chittleborough, D.J., Hutson, J.L. and B. Ostendorf (2009). Spatial heterogeneity of soil properties to predict pesticide movement. In: Ostendorf, B., Baldock, P., Bruce, D., Burdett, M. and P. Corcoran (eds.), *Proceedings of the Surveying & Spatial Sciences Institute Biennial International Conference*, Adelaide 2009, Surveying & Spatial Sciences Institute, pp. 1155-1165

Umali, B., Chittleborough, D., Ostendorf, B., Oliver, D., Huston, J., and Kookana, R. 2010. DEM and terrain analysis to predict spatial pattern of SOC. In: *Proceedings of the 19th World Congress of Soil Science: Soil solutions for a changing world*. 1-6 Aug 2010. Brisbane, Australia. Published on DVD.

### Conference Presentation

Umali, B., Oliver, D., Forrester, S., Ostendorf, B., Chittleborough, D., Huston, J., and Kookana, R. 2011. Spatial variability of diuron sorption in a hilly apple orchard. *ASA-CSSA-SSSA International Annual Meetings. Fundamental for Life: Soil, crop and environmental sciences*. 16-19 October 2011. San Antonio, TX (oral presentation).

*You have only to ask the cattle, for them to instruct you, and the birds of the sky, for them to inform you. The creeping things of earth will give you lessons, and the fish of the sea provide you an explanation: there is not one such creature but will know that the hand of God has arranged things like this! In his hand is the soul of every living thing and the breath of every human being!*

Job 12: 7-10