Modelling Agricultural Non-Point Source Pollution and Economic-Environmental Trade-Offs of Pollution Control Measures

A Project Overview

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This report forms part of a series of five reports, which are

i. GÖRGENS AHM, LORENTZ SA, VAN DER LAAN M, ANNANDALE JG, JOVANOVIC NZ, MATTHEWS N, GROVÉ B and LE ROUX JJ (2012). *Modelling Agricultural NPS Pollution and Economic-Environmental Trade-offs of Pollution Control Measures. A Project Overview.* WRC Report No. TT 516/12.
ii. VAN DER LAAN M, ANNANDALE JG, TESFAMARIAM EH, DU PREEZ CC, BENADÉ N, BRISTOW KL and STIRZACKER RJ (2012). *Modelling Nitrogen and Phosphorus Dynamics in Cropping Systems at the Field Scale*. WRC Report No. 1516/1/12.
iii. JOVANOVIC NZ, PETERSEN C, BUGAN RDH and VAN DER WALT E (2012). *Modelling the Fate of Pesticides: Primary Processes, Non-Point Source Data Collection and Guidelines.* WRC Report No. 1516/2/12.
iv. LORENTZ SA, KOLLONGEI J, SNYMAN N, BERRY SR, JACKSON W, NGALEKA K, PRETORIUS JJ, CLARK D and THORNTON-DIBB S (2012). *Modelling Nutrient and Sediment Dynamics at the Catchment Scale.* WRC Report No. 1516/3/12.
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EXECUTIVE SUMMARY

Background
Agriculture has been implicated, both locally and internationally, as a significant source of NPS pollution. Cognisant of this, the WRC initiated and funded a one-year scoping study in April 2003 to review the status of existing knowledge of agricultural NPS pollution and the related predictive modelling requirements and available tools. The review focussed on the following agriculture-derived NPS pollutants: phosphorus, nitrogen, pesticides, sediments, heavy metals and pathogens. The scoping study concluded with three deliverables, which included the terms of reference for the multi-year, multi-scale, multi-disciplinary project described in this overview report.

Project Objectives
The primary aim of the project was to develop an integrated modelling approach to prediction of agricultural NPS pollution from field- to catchment-scale for selected NPS pollutants. A secondary aim was to develop a modelling approach for examination of the economic-environmental trade-offs of agricultural pollution control measures, the effects of which were to be modelled by use of the field- and catchment-scale models. The specific objectives of the project stated in the original TOR were as follows:

- Establishment of fate-of-NPS-pollutant and other requisite data sets at field-, laboratory-, and quaternary catchment-scale, suitable for model improvement, development and verification.
- Improvement of understanding of on-farm NPS pollution control measures and their modelling requirements.
- Establishment of an improved field-scale model for simulation of agricultural NPS pollution loadings for phosphorus, nitrogen, selected pesticides and sediments, as well as for simulating the beneficial impacts on nearby receiving waters of on-farm NPS pollution control measures.
- Establishment of an improved quaternary catchment-scale model for simulation of agricultural NPS pollution loadings for phosphorus, nitrogen and sediments, as well as for simulating the downstream benefits of on-farm NPS pollution control measures at the catchment scale.
- Development of guidelines about model usage to examine economic trade-offs and feasibility of agricultural NPS pollution control measures at field- and catchment-scale.

Project Scope and Extent
The duration of the project was from April 2005 to February 2012 and involved researchers from nine different institutions and organisations: the Universities of Pretoria, the Free State, KwaZulu-Natal and the Western Cape, respectively, as well as the Agricultural Research Council (ARC), CSIR, SA Sugar Research Institute (SASRI), CSIRO (Australia) and Aurecon, who provided project leadership.

The Project was structured into four parallel but overlapping phases to ensure research effort synergies and inter-linked research outputs:

- Phase One: Observation and monitoring of NPS pollution processes at point-, field- and catchment-scales (nutrients, sediments and pesticides).
- Phase Two: Developing field-scale NPS pollution predictive capability via a bio-physical field-scale model (nutrients and sediments), as well as an expert system (pesticides).
- Phase Three: Developing catchment-scale NPS pollution predictive capability via catchment-scale bio-physical models (nutrients and sediments).
- Phase Four: Developing economic-environmental trade-off modelling ability, supported by the above bio-physical models.

Technology Transfer

The project yielded five published final reports: this overview report and four detailed technical accounts of the research on the field-scale bio-physical modelling, the field-scale expert system for pesticides, the catchment-scale modelling and the economic-environmental trade-off modelling, respectively. The project also yielded 14 journal papers and presentations at conferences and symposia and at least three more are in progress. This overview report is not a detailed scientific presentation of the research conducted during this project. The research details are documented in depth in the four sister-reports referred to above. Instead, we present here a narrative overview of the study, its challenges, its achievements and its learnings in the hope that a wider audience would find it accessible and useful.

Capacity Building

Given the research nature of the project, as well as the involvement of a number of academic and research institutions, a large capacity building component was maintained throughout and the project supported 13 post-graduate students.

Project Team Composition

The project team was composed of four individual task teams, comprising one or more specialists within each of the domains of agricultural nutrients, sediments, pesticides, field-scale bio-physical modelling, catchment-scale bio-physical modelling, and agricultural economics. As stated earlier, the specialists were drawn from a range of academic and research institutions. The research consulting firm, Sigma Beta, was appointed to provide leadership, coordination and administration to the research team. In 2009 Sigma Beta was absorbed into Aurecon, a global professional consulting firm, who continued with the leadership role previously performed by Sigma Beta.

Task Team: Nutrients and Field-Scale Modelling

Data collection

For field-scale nitrogen (N) and phosphorus (P) model testing and validation purposes, a range of historical datasets were scrutinized, after which three datasets were judged appropriate. These datasets were collected in the Netherlands, Kenya and South Africa, and were selected according to suitability, primarily based on the scale at which the data was collected and the variables involved.

Development of SWB-Sci, a field-scale nitrogen and phosphorus crop model

SWB-Sci is a mechanistic, generic crop model originally developed at the University of Pretoria in South Africa as a real-time irrigation scheduling tool. Evapotranspiration is calculated according to the Penman-Monteith grass reference method. During recent years extensive crop parameterization work had been done for SWB-Sci and validation exercises had shown that the model can representatively simulate the soil-plant-atmosphere continuum.

As part of this project, N and P subroutines have been included into the existing SWB-Sci model. Wherever practicable, algorithms from well-established existing models were used. During the model development phase it became clear that obtaining P initialization soil parameters for South African soils was highly challenging; consequently, the Team developed specific guidelines to assist model users in the parameterization of South African soils. The guidelines were published as a scientific paper – Van der Laan et al. (2009) – and enable catchment-scale modellers to utilize land type maps, which are available for the whole of South Africa at a scale of 1:250 000, to parameterize models.

During model testing with the datasets from the Netherlands and South Africa, the model was judged to simulate N dynamics in cropping systems more than adequately. The newly introduced approach to simulate the effect of N stress on yield on a daily basis following flowering, as opposed to simulating the effect of N stress on the harvest index as used in older models, proved to be effective.

Demonstration of field-scale nutrient pollution mitigations/controls
Long-term simulations with SWB-Sci were conducted to compare leaching losses from a dryland and an irrigated cropping system and to assess the effectiveness of different on-field pollution mitigation measures for the irrigated system. Data from a field trial conducted in the Free State, South Africa, was used to initialize and calibrate the SWB-Sci model.

Annually, N leaching was estimated to be 433% higher for an irrigated system compared with a dryland system. A split-application for fertiliser led to higher mean annual N leaching than for the single application case. A ‘room for rain’ irrigation strategy was able to reduce N leaching by 11%, while a crop rotation strategy reduced N leaching by 42%. Employing a crop rotation practice as well as a ‘room for rain’ irrigation strategy simultaneously reduced N leaching most effectively (58%). Nevertheless, this strategy still led to N leaching 182% above that estimated for the dryland system. These results demonstrate that field-scale pollution mitigation measures can significantly reduce N leaching from irrigated agriculture, but not to levels observed for dryland production.

Task Team: Pesticide Modelling
Data collection
As part of the Pesticides Task, a nested, experimental catchment was established in the Western Cape, South Africa, in the vicinity of Riebeek-West, on the farm, Goedertrou. The point- and field-scale was represented by two standard Wischmeier runoff plots (22.3 m x 2 m) established at the beginning of observations in 2005. The small-catchment-scale responses were represented by the farm dam collecting water from the Goedertrou catchment, which is approximately 20 ha in area. The crop rotation was one season of dryland wheat followed by two years of fallow land to regenerate soil fertility and for re-growth of previously cultivated pasture grasses. The following data were collected: hourly and daily weather data; wheat yield; re-growth of grasses on fallow land; hourly volumetric soil water contents at two depths and positions in the soil profile; overland flow from the runoff plots, including sampling for laboratory analyses of pollutants; pesticide concentrations in soil and runoff water and in the dam; nutrient (N and P) concentrations in the soil root zone and runoff water; sediments mobilized from the runoff plots; water level in the dam; and geological, elevation and soils mapping.

Development of Pesticide Environmental IndeX (PestEX)
One of the first activities carried out in the Pesticide Task was to identify priority processes and variables for pesticides in order to improve/augment existing models/methods applicable to different scales, as well as pesticide mitigation/control measures. Numerous process models available internationally can simulate the priority pesticide processes identified in this project. However, the application of process models to predictions of pesticide impacts on water resources presents serious challenges. Some of the challenges are the complexity of the soil-plant-atmosphere system; large extent and intensity of input data required; large number of chemicals available on the market with specific properties; lack of knowledge on pesticide behaviour, toxicity and temporal uncertainties; and infeasibility and expense of intensive monitoring for a large number of pesticides.

Given these challenges, the pesticide team decided to develop PestEX, an expert system for modelling the fate of pesticides at field-scale. The Pesticide Environmental IndeX (PestEX) is an Excel-based calculator that accounts for the main factors affecting the contamination of surface- and groundwater, namely pesticide drift, position of application in relation to streams and groundwater, general slope of the area, dominant flow direction (vertical or horizontal), tillage practices, soil hydraulic properties, irrigation practices/rainfall distribution, pesticide properties (volatilization, sorption and degradation), pesticide application and sensitivity of the receiving water resource.

The novelty of the approach is that the factors were combined based on their occurrence at different scales. Mitigation/control measures (wetlands, buffer strips and contours) are also considered to be factors in the calculation of environmental mobility of pesticides. Each factor is scored (rating x weighting) to produce a combined environmental score. Pesticide application is used to calculate an economic score corresponding to pollution abatement costs. Fuzzy logic normalization of the factors allows comparison and minimization of environmental and pollution abatement costs.

Being written in Excel, PestEX is easy to use and interactive. An Excel worksheet is dedicated to the input and calculation of each influential factor and it can be accessed by clicking on the relevant command button in the Main Menu (main worksheet). Any factor can be disabled by clicking on tick-boxes. The programme makes extensive use of pop-up comments to facilitate the user in operating as well as selecting the inputs. Links to databases, reviews and references are available within the programme. The graphs are interactive and they automatically show input data and ratings for each factor.

Task Team: Catchment-Scale Modelling

Data collection

As part of the Catchment-Scale Task, the Mkabela nested, experimental catchment was established in a sugar cane growing area in KwaZulu-Natal, South Africa, in order to examine the migration processes of nutrients from the field-scale to the catchment-scale, through surface and subsurface pathways to receiving waterways, as well as through the controls and links affecting the pollutant fate. The catchment monitoring was designed to enable detailed observations in a small headwater sub-catchment, with nested sampling points at progressively increasing contributing areas. Catchment-scale observations comprised continuous flow monitoring as well as periodic sampling for nutrients and sediments at selected stations representing increasing catchment areas.

Overland, subsurface and in-stream water, nutrient and sediment processes were observed, while intermittent discharge measurements were made and water samples taken at the nested stations, including two Wischmeier runoff plots. Comprehensive soil and land use surveys were completed and the main stream network was surveyed and described. The land use in the catchment comprised primarily sugar cane, but with scattered areas of forestry, vegetables, maize, pastures, wetlands and farm dams. Soil water tension was logged in the profiles and cores were extracted during selected wet and dry periods for soil nutrient analysis.

The ACRU-NPS model

ACRU is a deterministic agrohydrological model – developed in South Africa – based on the SCS algorithm that simulates daily discharge and peak runoff from daily rainfall. Sediment yield per unit area from a land unit is based on the Modified Universal Soil Loss Equation (MUSLE) in which the energy for sediment entrainment and transport is derived from the event discharge volume and peak flow rate and empirical soil erodibility, vegetative cover, slope and practice factors determine the sediment yield. Inclusion of nutrient mass balance algorithms in *ACRU* enabled simulation of N and P losses in surface runoff, sediment, and leaching; N and P cycling in the soil-water-plant-animal system; and N and P mass balances in the catchment system. The resultant "*ACRU-NPS"* includes rainfall, irrigation, fertilisers, plants, and animal wastes as potential nutrient sources and simulates pollution management impacts on N and P transformations and transport. The most recent version of functions in the GLEAMS model was used as a guide in the development of *ACRU-NPS*. New components and processes added to *ACRU* were a plant residue layer, a soil surface layer, plant matter removed, soil temperature, ammonification, nitrification, N plant uptake and fixation, volatilisation, denitrification, N adsorption and extraction, ammonium partitioning, immobilization, P mineralisation, P plant uptake, P adsorption and extraction, labile P partitioning, harvest, tillage, surface and evaporation transport, subsurface transport and crop stress recovery after moisture or nitrogen shortfalls.

An important aspect of this task was the development of comprehensive guidelines for the catchment-scale parameterisation of nutrient-affecting processes based on current laboratory- and field-scale research. Close interaction with the SWB-Sci development team played a major role in the successful completion of this aspect.

ACRU-NPS was configured in detail for the Mkabela catchment and simulated values of NO_3, P and suspended solids were compared with observed values. The simulated NO_3 loads corresponded well with those observed, while the simulated P loads were lower than observed. Subsurface delivery of water and possibly P was poorly simulated, which could be the reason for the low simulated P concentrations. Simulated sediment loads were higher than observed during the wet season. The sensitivity of the soil erodibility to simulated antecedent water content may be the reason for over-simulation of sediment loads during wet periods.

With the above *ACRU-NPS* modifications completed, a series of scenarios were analysed using a 50-year daily rainfall sequence. For the purpose of the scenario modelling, the catchment model was re-configured as a simplified network of land segments based on the dominant land use, as well as on the in-stream and riparian network controls and buffers.

The scenarios comprised:

- *Base case:* current land use (including contours);
- *No contours:* current land use, but no contours used in the sugar cane segments;
- *All sugar:* all land uses set to sugar cane (including contours);
- *Irrigation:* current land use, but with deficit irrigation applied to the sugar cane;
- *No buffers:* Base scenario, but with on-farm controls (farm dams and buffers) removed.

All these scenarios were run with a series of fertiliser applications, comprising current fertilization practice (Base), twice, half and quarter of the Base fertiliser applications and finally, zero fertiliser. The resulting simulated sediment and nutrient loadings into and out of the significant in-stream controls – the three large wetlands and the two large dams – were analysed comparatively for all these scenarios, as were sugar cane yields. The comparative results indicate significant pollution benefits or aggravating pollution loads linked to particular scenarios.

The SWAT model

SWAT is a catchment-scale model that was developed in the USA to predict the impact of land management practices on water, sediment, and agricultural chemical yields on complex landscapes with varying soils, land use, and management conditions over long periods of time. The intention was not to improve and augment SWAT as was done with *ACRU-NPS*; rather, the intention was to provide a comparative catchment-scale alternative to *ACRU-NPS*.

SWAT is based on a modified SCS algorithm. Sediment yield is computed with the MUSLE algorithm and loading functions estimate the daily organic N/P runoff loss based on the concentration of organic N/P in the top soil layer, the sediment yield, and enrichment ratio. Once the runoff and loads sediment and nutrients have been determined for all specified sub-catchments, SWAT routes the loads through the stream network of the catchment. Flow is routed through the channel using a variable storage coefficient method and sediment is routed by means of stream power theory. Nutrients are routed through the channel using equations from the QUAL2E model, whereby the model tracks nutrients dissolved in the stream and nutrients adsorbed to the sediment. The crop growth and yield component of SWAT is a simplified version of the EPIC plant growth model.

SWAT was configured in detail for the Mkabela catchment and simulated values of NO_3, P and suspended solids were compared with observed values. Compared to observed values, SWAT successfully tracked most of the peak flow events that occurred during the year, although the peaks were usually over-predicted. In contrast, the majority of the low-flow periods were slightly under-predicted. Sediment concentrations for peak flow events were usually under-predicted, whereas the sediment concentrations for the majority of the low-flow periods were slightly over-predicted. A possible cause of the above outcomes could be unrepresentative trap efficiencies of the nine farms dams as simulated by SWAT in the Mkabela catchment. For example, small dams seem to have similar trap efficiencies to dams a hundred times larger in area.

In comparison with *ACRU-NPS*, the SWAT-simulated annual average pollution loadings in the Mkabela catchment were low. Primary causes of these discrepancies are likely to be different model representations of site-specific processes of overland versus subsurface discharge and nutrient flux. SWAT seems to incorporate adequately the physics of important hydrological structures, such as wetlands, farm dams and channel roughness. Furthermore, the GIS-interfaces of SWAT were efficiently configured to include all the nested sub-catchments in the large catchment. The simulation of loads at multiple scales in the large catchment allowed easy interrogation of the effect of controls such as wetlands, riparian buffers and farm dams on the progress of pollutants downstream.

The relative impacts of eight alternative pollution management scenarios in terms of flow, sediment and nutrients at the outlet to the Mkabela catchment were examined using the SWAT model. The scenarios comprise the whole catchment under, respectively, sugar cane; vegetables with soil being tilled; vegetables with no till practices; current cover and practices with zero nutrients added; current cover and practices with 50 kg/ha mineral P and 100 kg/ha mineral N applied; current cover and practices with double nutrients applied; current cover and practices, but excluding all wetlands; current cover and practices with 1.5 m buffer strips surrounding cultivated fields. The comparative results indicate significant pollution benefits or aggravating pollution loads linked to particular scenarios.

Task Team: Economics of Agricultural NPS Pollution Management

Trade-off model development

For this Task a state contingent approach was used to characterise pollution risk during crop production. State contingent theory suggests that a production function or pollution loading function exists for every state of nature, e.g. every year or production cycle would have a different function due to the effect of weather on production. To this end simulation results from both SWB-Sci and *ACRU-NPS* were used to fit crop production functions, irrigation-fertiliser response functions and pollution loading functions for each production cycle. These functions were combined with economic data to estimate the margin above specified cost (MAS) for particular production scenarios.

Pollution load distributions cannot be generic, due to the site-specific nature of agricultural NPS pollution. To overcome the problem of specifying the distributional form, an upper partial moment (UPM) approach, based on an empirical distribution, was developed. The UPM model treats pollution loads as an empirical distribution and determines a target pollution level endogenously, based on a user-specified environmental goal.

To determine the economic-environmental trade-offs when maintaining environmental standards, two optimisation models were developed. The first model determines the optimal MAS with no constraint on pollution emissions. The results are then used to determine the baseline pollution level, which is then constrained in the second model to determine environmental compliance according to user-specified pollution "targets" (or standards). Economic-environmental trade-off curves were developed by solving the compliance model and maximising MAS for different levels of pollution abatement.

Economic-environmental trade-off case studies
Three case studies were undertaken to examine the trade-offs between economic benefits versus costs and water quality-related environmental benefits versus costs of agricultural pollution control measures at field-scale, farm-scale and catchment-scale, respectively.

For the field-scale analysis of economic-environmental trade-offs the SWB-Sci model was used to generate crop production-related information for irrigated late-monoculture maize in the Free State Province of South Africa. Production functions and pollution loading functions were developed for four scenarios: two different soils (sandy clay loam and sandy clay) and two different management practices (split versus single application of fertilisers), respectively. Optimal irrigation water use associated with the production of maize was simulated, thus the crop did not experience water stress during any stage of production. Production values were simulated for 18 production years between 1981 and 2000. Trade-off curves were developed for the four scenarios, respectively.

For the farm-scale analysis of economic-environmental trade-offs the SWB-Sci model was also used to generate crop production-related information for irrigated late-monoculture maize for the above 18 production years. The cultivatable soils mix of the farm was assumed to be 60 ha SCL and 30 ha SC. Only single fertiliser applications were specified.

For the catchment-scale application, *ACRU-NPS* was used to simulate the runoff and pollution from, as well as the crop production in, the Mkabela catchment. Production practices were varied on the sugar cane areas only, while the rest of the areas were assumed to remain unchanged. Five alternative fertilisation regimes for sugar cane were super-imposed on the model. The fertiliser regime recommended by SASRI was taken to be the Base regime. Alternative fertiliser regimes were half, quarter and double the recommended regime, as well as zero fertiliser. The fertiliser applications consisted of organic and inorganic fertiliser.

Production-related model outputs were generated for a period of 50 years with a production cycle of 18 months for sugar cane production, with and without field contours and buffers. Meta-models in the form of "contribution coefficients" were used to represent reductions in pollution loads as they move through the controls (i.e. buffers, dams and wetlands). The pollutant loads from the land segments, associated crop yields and contribution coefficients were used in a spatial network node optimisation model to determine economic-environmental trade-offs.

Typical results
As illustration of typical results, the economic-environmental trade-off curves developed for the four field-scale scenarios are depicted in Figure EX.1 for a pollution output compliance assurance/probability of 90% and for incrementally more stringent environmental targets. For example, for the environmental target, Target_10, this means that during 90% of production years the N pollution output level is constrained to be 10% less than the average values determined in the Baseline case (the maximised MAS case). The drastic MAS drop between the Baseline and Target_0 may be interpreted as the "cost" of having to implement on-field mitigations to limit pollution output exceedences of the "average" levels of the Baseline case to less than 10% of production years.

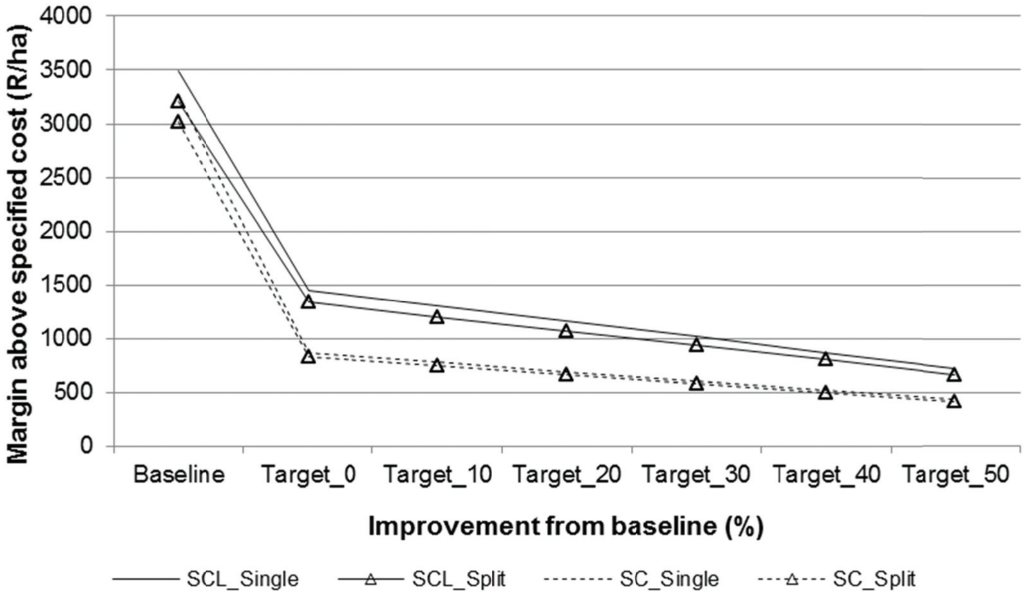

Figure EX.1: Field-scale economic-environmental trade-offs for a 90% compliance probability on a sandy clay loam and sandy clay soil with a single and split fertiliser application.

Comparable economic-environmental trade-off curves were developed for the farm-scale and catchment-scale scenarios.

Lessons Learnt

In this section of the overview report each team outlined the new understandings, insights and learnings about multi-scale, multi-disciplinary research processes and concepts that were attained during the project. The following headings were used to group the responses:

- Overarching project Learnings
- Research design
- Approaches to scaling
- Multi-Team/Multi-Location integration and collaboration
- Interfacing natural resource management needs and scientific realities

In total, six overarching "project learnings", as well as 28 individual task team "lessons learnt", were formulated.

Further Research Recommendations

In this section of the overview report each team outlined further research recommendations to cover the scientific, technical and data shortcomings and gaps experienced during the execution of their task, as well as to take specific aspects of their individual methodologies and models to a higher level. A total of 29 individual research recommendations were formulated by the four teams.

The Way Forward

In this section of the overview report a follow-up research project of a long-term, multi-scale, trans-disciplinary nature is proposed to encapsulate the above "lessons learnt" and "further research recommendations" in a systematic, integrated manner, and in full cognisance of relevant recent local and international research developments. This follow-up project would need to include ongoing broad engagement by the research team with farmers, agricultural extension officers, officials in regulatory roles, agricultural and environmental planning officials, related policy-makers and related NGOs.

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The members of the Reference Group were as follows:

Dr K Bristow	CSIRO, Australia
Mr M du Plessis	Water Research Commission
Dr R Heath	Golder and Associates
Dr M Ligthelm	Department of Water Affairs
Prof M Lord	University of Western Carolina
Mr T Matsetela	NAFU
Prof J Miller	University of Western Carolina
Ms A Nefale	Department of Water Affairs
Mr N Opperman	Agri SA
Ms L Ramashala	Department of Water Affairs
Mr R Ranwedzi	Department of Water Affairs
Prof C Reinhardt	University of Pretoria
Dr H Sally	CGIAR
Mr K Taylor	Department of Agriculture, Forestry and Fisheries

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We owe a special word of gratitude to Ms Simone Lyons for her professional coordination and administration of this project.

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1 INTRODUCTION

It is well recognised that non-point source (NPS) pollution plays a major role in the degradation of water quality, particularly with regard to nutrients and suspended sediments. It is furthermore increasingly accepted that it is infeasible to manage catchment water quality without addressing the contribution from non-point sources. Consequently, energy is increasingly devoted to the quantification of NPS pollution in catchments and to identify means to control it cost-effectively.

Agriculture has been implicated, both locally and internationally, as a significant source of NPS pollution. Water quality concerns that can be related to NPS impacts of agricultural activities include: *salinisation* (through irrigation return flows or salt wash-off and leaching under dry-land cultivation); *eutrophication* (through fertiliser leaching and nutrient wash-off from human settlements on farms); *sediments* (as a result of erosion); *pathogens* (from intensive animal production units and poorly sanitised settlements on farms); *pesticides* (through the application of insecticides, fungicides and herbicides); and *heavy metals*.

During 2001 the Water Research Commission (WRC) published a Guide for non-point source assessment for use in catchment water quality management processes (Pegram and Görgens, 2001). This Guide was intended to assist water quality practitioners to identify and apply generic NPS assessment techniques; however, it did not include any direct model development and testing, nor did it deal with the agricultural sector specifically. The Guide identified discrete research needs, the outcomes of which would enhance the usefulness of a number of proposed methodologies in the Guide. These included: researching the production, delivery, transport and use of agriculture-derived NPS loadings in water resources, and developing a predictive ability regarding the fate of agriculture-related NPS pollution constituents.

At the time of the publication of the Guide, research related to the links between crop farming and *salinisation* had been funded by the WRC for many years, but research into agriculture's contribution to the other water quality concerns had not attained the same degree of attention.

Cognisant of the above, the WRC initiated a one-year Scoping Study in April 2003 to review the status of existing knowledge of agricultural NPS pollution and the related predictive modelling requirements and available tools. The review focussed on the following agriculture-derived NPS pollutants: phosphorus, nitrogen, pesticides, sediments, heavy metals and pathogens. The Scoping Study concluded with the following three deliverables:

(i) *Knowledge Review of Modelling Non-Point Source Pollution in Agriculture from Field to Catchment Scale (Rossouw, Cullis and Görgens, 2004).*

(ii) *First Order Estimate of the Contribution of Agriculture to Non-Point Source Pollution in Three South African Catchments: Salinity, Nitrogen and Phosphorus (Cullis, 2004).*

(iii) *Terms of Reference (TOR) for a multi-year, multi-disciplinary project which was to focus on fundamental, applied and integrated research to develop the required knowledge and skills to model NPS pollution from agriculture at spatial resolutions that range from field- to catchment-scale and to model the economic trade-offs of agricultural pollution control measures.*

In 2005, the WRC appointed the multi-disciplinary Research Team described in Section 4.1 to undertake the latter Project, under the WRC's Key Strategic Area – Water Utilisation in Agriculture; Thrust 4: Water Resource Protection and Reclamation in Agriculture.

2 PROJECT OBJECTIVES, SCOPE AND METRICS

2.1 Objectives

The primary aim of the Project was to develop an integrated modelling approach to prediction of agricultural NPS pollution from field- to catchment-scale for selected NPS pollutants. A secondary aim was to develop a modelling approach for examination of the economic-environmental trade-offs of agricultural pollution control measures, the effects of which were to be modelled by use of the field- and catchment-scale models. The specific objectives of the Project stated in the original TOR were as follows:

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- Improvement of understanding of on-farm NPS pollution control measures and their modelling requirements.
- Establishment of an improved field-scale model for simulation of agricultural NPS pollution loadings for phosphorus, nitrogen, selected pesticides and sediments, as well as for simulating the beneficial impacts on nearby receiving waters of on-farm NPS pollution control measures.
- Establishment of an improved quaternary catchment-scale model for simulation of agricultural NPS pollution loadings for phosphorus, nitrogen and sediments, as well as for simulating the downstream benefits of on-farm NPS pollution control measures at the catchment scale.
- Development of guidelines about model usage to examine economic trade-offs and feasibility of agricultural NPS pollution control measures at field- and catchment-scale.

2.2 Scope and Extent

The duration of the Project was from April 2005 to February 2012 and involved researchers from nine different institutions and organisations: the Universities of Pretoria, the Free State, KwaZulu-Natal and the Western Cape, respectively, as well as the Agricultural Research Council (ARC), CSIR, SA Sugar Research Institute (SASRI), CSIRO (Australia) and Aurecon. These researchers are identified in Section 4.1.

The Project was structured into four parallel but overlapping phases to ensure research effort synergies and inter-linked research outputs:

- Phase One: Observation and monitoring of NPS pollution processes at point-, field- and catchment-scales (nutrients, sediments and pesticides).
- Phase Two: Developing field-scale NPS pollution predictive capability via a bio-physical field-scale model (nutrients and sediments), as well as an expert system (pesticides).
- Phase Three: Developing catchment-scale NPS pollution predictive capability via catchment-scale bio-physical models (nutrients and sediments).
- Phase Four: Developing economic-environmental trade-off modelling capability, supported by the above bio-physical models.

2.3 Technology Transfer

The Project yielded five published final reports: this Overview Report and one each on the field-scale bio-physical modelling, the field-scale expert system for pesticides, the catchment-scale modelling and the economic-environmental trade-off modelling. The full titles of the five final reports are as follows:

i. GÖRGENS AHM, LORENTZ SA, VAN DER LAAN M, ANNANDALE JG, JOVANOVIC NZ, MATTHEWS N, GROVÉ B and LE ROUX JJ (2012). *Modelling Agricultural NPS Pollution and*

Economic-Environmental Trade-offs of Pollution Control Measures. A Project Overview. WRC Report No. TT 516/12.

ii. VAN DER LAAN M, ANNANDALE JG, TESFAMARIAM EH, DU PREEZ CC, BENADÉ N, BRISTOW KL and STIRZACKER RJ (2012). *Modelling Nitrogen and Phosphorus Dynamics in Cropping Systems at the Field Scale*. WRC Report No. 1516/1/12.

iii. JOVANOVIC NZ, PETERSEN C, BUGAN RDH and VAN DER WALT E (2012). *Modelling the Fate of Pesticides: Primary Processes, Non-Point Source Data Collection and Guidelines.* WRC Report No. 1516/2/12.

iv. LORENTZ SA, KOLLONGEI J, SNYMAN N, BERRY SR, JACKSON W, NGALEKA K, PRETORIUS JJ, CLARK D and THORNTON-DIBB S (2012). *Modelling Nutrient and Sediment Dynamics at the Catchment Scale.* WRC Report No. 1516/3/12.

v. MATTHEWS N and GROVÉ B (2012). *Modelling Economic-Environmental Trade-Offs of Agricultural Non-Point Source Pollution Control Measures*. WRC Report No. 1516/4/12.

Furthermore, at the time of writing the Project had already yielded 14 journal papers and presentations at conferences and symposia, with at least three more papers in the pipeline. The completed papers are referenced in Appendix A.

2.4 Capacity Building

Given the research nature of the Project, as well as the involvement of a number of academic and research institutions, a large capacity building component was maintained throughout and the Project supported four PhD students, seven Master's students, one honours student and one post-doctoral research fellow. Their details are provided in Appendix B.

3 PROJECT AND REPORT FRAMEWORKS

3.1 Project Framework: FAIM Knowledge Management Hierarchy

The provision of support to management decision-making is an important end-goal of many research undertakings that focus on natural resources. In its generic sense, management encompasses the interactive cycle of information assembly, assessment, policy formulation, planning, option analysis, prioritisation, implementation, operation, monitoring, auditing and correction. The quality of support to management decision-making depends on sound linkages between an understanding of bio-physical processes at different scales, as well as on the integration of bio-physical with other forms of knowledge. These requisite linkages are the keys to an interactive, overlapping hierarchical structure of knowledge and the layers of research, methodologies and tools that feed knowledge-generation. For convenience, this structure can be called the FAIM (*Fundamental/ Applied/ Integrative/ Management Support*) knowledge generation and management framework – illustrated in **Figure 3.1**.

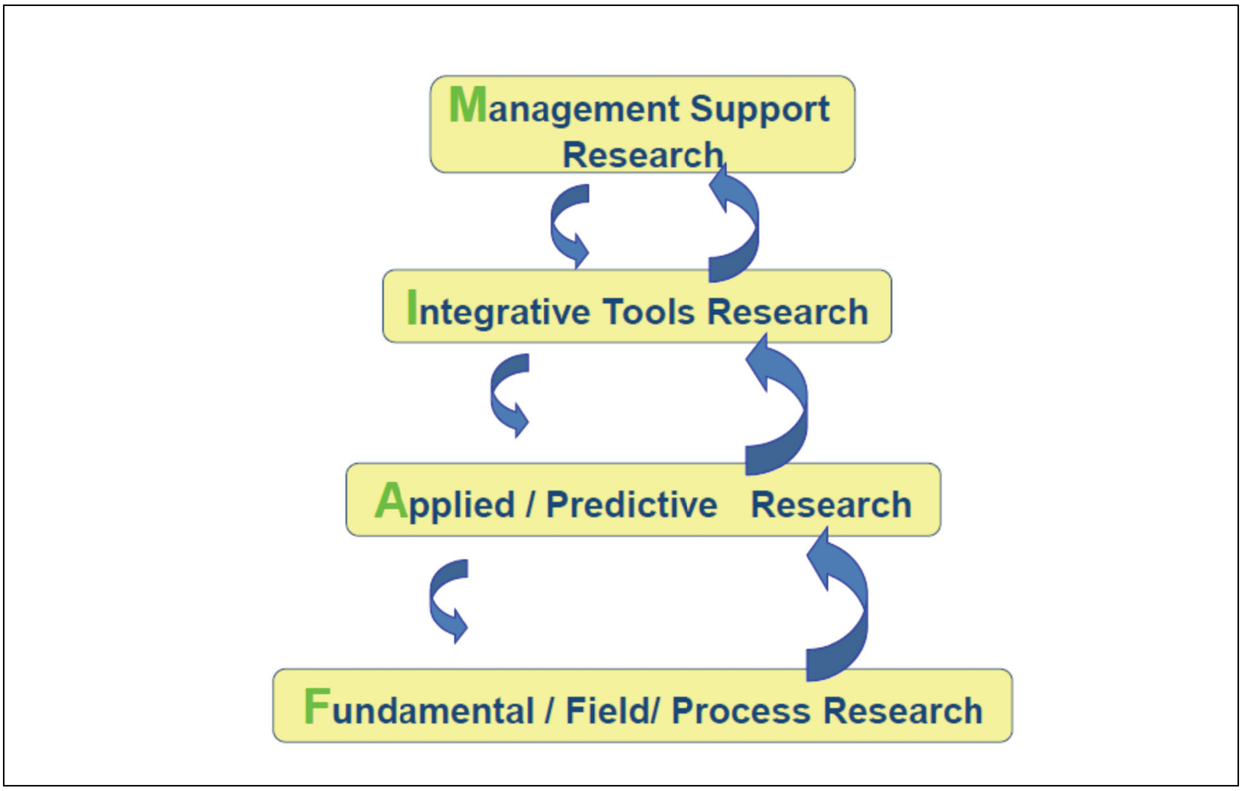

Figure 3.1: FAIM Knowledge Management Framework

The FAIM framework provides structure to the analysis and evaluation of knowledge generation and management in a particular domain as follows:

- Key research or management questions, relevant to each of the FAIM levels, are linked to the knowledge-generation processes at that level.
- Methodologies and tools used in research, or process quantification, or spatial and temporal extrapolation, or impact assessment are juxtaposed to each of the requisite levels.
- Existing or new understanding is recorded and organised in a systematic manner, with retention of cross-linkages.
- Knowledge gaps are accurately identified through in a holistic understanding of the knowledge-generation process.

- Research needs can be focused at particular FAIM levels, thereby facilitating efficiency in research efforts.

The FAIM framework was made applicable to the design of this Study, as follows: The research questions relating to the generation, transport and transformation of NPS pollutants due to agriculture, as well as the scientific challenges relating to NPS pollution prediction and the use of such prediction to support management decision-making, were appropriately linked to relevant FAIM levels and informed the knowledge-generation processes at the applicable levels. In more specific terms, this entailed the following:

- FAIM level 1 – *fundamental*: observation, measurement and monitoring of individual NPS pollution processes at a range of scales and the derivation of conceptual algorithms for individual NPS components or localised NPS responses
- FAIM level 2 – *applied*: extrapolation and up-linking from individual NPS pollution process component concepts (a) to full generic bio-physical process models with coupled algorithms that enable nutrient water quality prediction at point- and field-scales, and (b) to an expert system for pesticide dynamics at field scale
- FAIM level 3 – *integrative*: integration of numerous NPS pollution processes across various scales into a range of bio-physical sub-models that, closely-coupled, enable nutrient and sediment water quality prediction at catchment-scale
- FAIM level 4 – *management support*: developing economic-environmental trade-off analysis tools that are loosely coupled with bio-physical model simulations of the effects of NPS pollution control measures.

The design of the four Project Phases outlined in Section 2, was informed by the four levels of the FAIM knowledge management hierarchy.

It should be noted that, operating across the FAIM levels, were individual Specialist Task Teams, respectively focusing on nutrients, sediments, pesticides, field-scale modelling and catchment-scale modelling. These Research Teams are described in Section 4.

3.2 Overview Report Approach and Framework

This Overview Report is not a detailed scientific presentation of the research conducted during this Project. The research details are documented in depth in the four sister-reports referenced in Section 2.3. Instead, we present here a narrative overview of the Study, its challenges, its achievements and its learnings in the hope that a wider audience than that of the sister-documents would find it accessible and useful.

This Overview Report has been broadly structured according to the FAIM framework, but for ease of presentation, the overview of each Task Team’s contributions to the relevant FAIM levels is presented as separate sections.

4 PROJECT TEAM AND THE CHALLENGE OF INTEGRATION

4.1 Structure of the Project Team

The Project Team was composed of four individual Task Teams, comprising one or more Specialists within each of the domains of agricultural nutrients, sediments, pesticides, field-scale bio-physical modelling, catchment-scale bio-physical modelling, and agricultural economics. As stated earlier, the Specialists were drawn from a range of academic and research institutions. The research consulting firm, Sigma Beta, was appointed to provide leadership, coordination and administration to the Research Team. In 2009 Sigma Beta was absorbed into Aurecon, a global professional consulting firm, who continued with the leadership role performed by Sigma Beta.

The original structure of the Project Team, as presented in the Project Proposal, is shown in the Organogram in **Figure 4.1**.

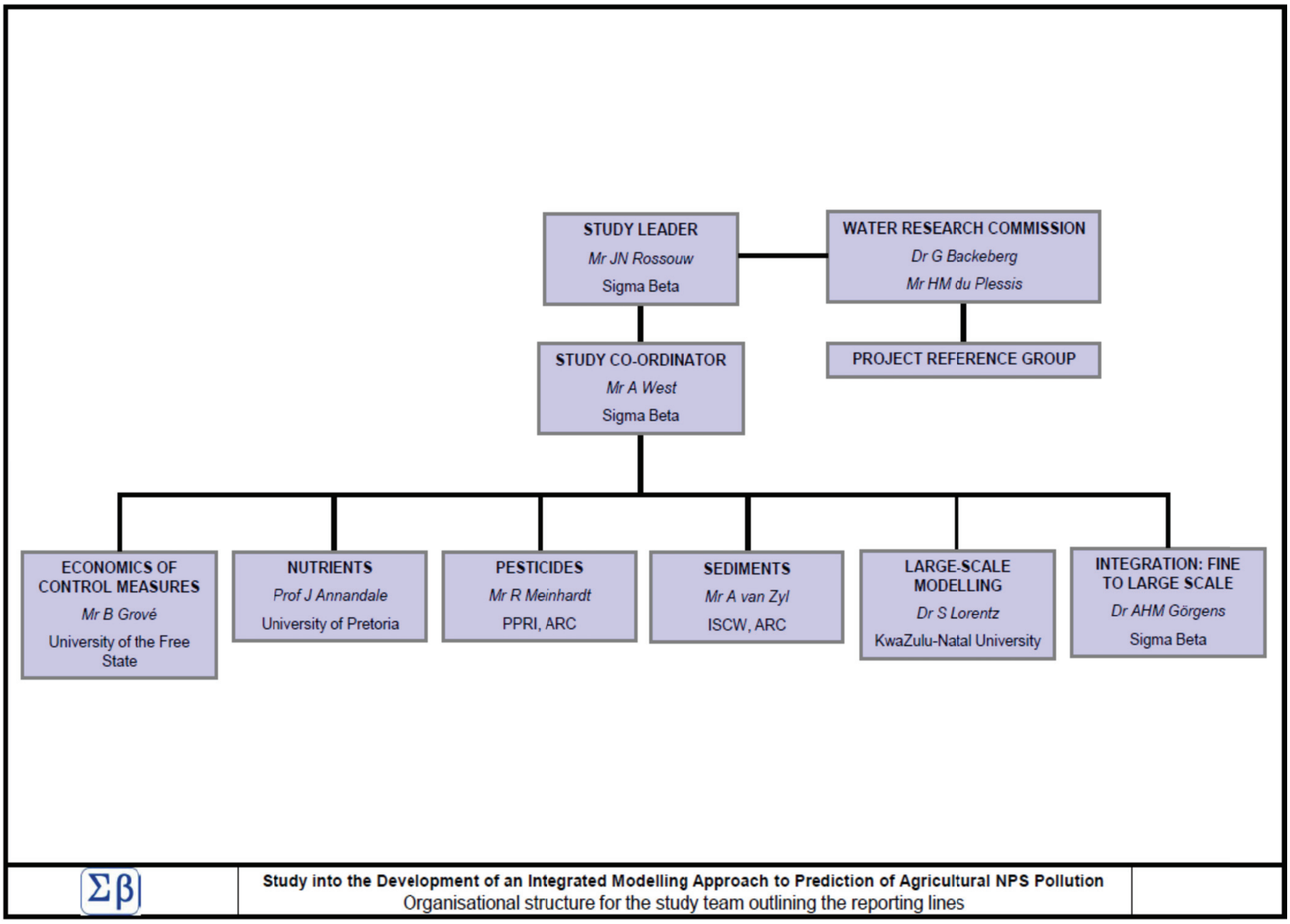

Figure 4.1: Project Organogram

As with most multi-year projects, changes within the Team make-up over time were inevitable. During the life of this Project, the following changes occurred:

- In March 2005, **Mr Albert van Zyl**, of the Agricultural Research Council (ARC), Institute for Soil, Climate and Water, was replaced by Mrs Talita Germishuyse, as the *Task Leader: Sediments.*

- In April 2008, **Mr Nico Rossouw** of Sigma Beta was replaced by **Prof André Görgens** as *Study Leader*.

- In April 2008, **Mr Ashwin West** of Sigma Beta was replaced by **Ms Simone Lyons** as *Study Coordinator*.

- In January 2009, **Mrs Talita Germishuyse** of the Agricultural Research Council, Institute for Soil, Climate and Water, was replaced by **Mr Jay Le Roux** as the *Task Leader: Sediments.*

- In November 2007, **Dr Nebo Jovanovic,** *Task Leader: Pesticides*, changed his employment from the University of the Western Cape, Earth Science Department, to the CSIR, Hydroscience Group, Natural Resources and Energy (NRE). After his move he continued with his role as Task Leader.

The Task Leaders who remained in their position throughout the life of the Project were the following:

- **Prof John Annandale**, of the University of Pretoria, Plant Protection and Soil Science Department – *Task Leader: Nutrients.* This Task included *Point- and Field-Scale Modelling.*

- **Dr Simon Lorentz**, of the University of KwaZulu-Natal, School of Bioresources Engineering and Environmental Hydrology – *Task Leader: Large-Scale Modelling*

- **Dr Bennie Grové**, of the University of the Free State, Department of Agricultural Economics – *Task Leader: Economics of Agricultural NPS Pollution Management & Control Measures.*

4.2 Challenge of Integration

Alignment, coordination, integration and consistent administration are predictable challenges in multi-disciplinary projects – more so when the respective teams are spatially and institutionally remote from each other. In order to meet these challenges, the following two roles were included in the Project Team:

- *Integration Task Leader*: The specific focus of the Integration Task was the facilitation of the integration of the individual scientific contributions into a common bio-physical modelling approach that would bridge finer and coarser spatial scales, as well as shepherding the interface between the Economics Team and the Bio-physical Modelling Teams. During the life of the Project this Task comprised the organisation and facilitation of four annual Task Team Workshops, three joint field visits and more than a dozen mini-workshops and brainstorming sessions in which sub-groupings of the respective Research Teams participated. Prof André Görgens of Sigma Beta/Aurecon led this Task.
- *Study Coordinator*: This role comprised the continuous day-to-day coordination, monitoring, routine correspondence, financial management and administration tasks, performed under the supervision of the Study Leader.

5 OUTCOMES AND OUTPUTS

5.1 Team: Nutrients and Field-Scale Modelling (Van der Laan et al., 2012)

5.1.1 *Fundamental Process and Field Research*

Quantifying nitrogen (N) losses in deep drainage is highly challenging due to uncertainties in estimating drainage fluxes and solute concentrations in the leachate. Active and passive soil water samplers are used to determine solute concentrations and estimate leaching, but give limited information on water fluxes. Mechanistic models are also used to estimate leaching, but often require complex calibration with measured data to ensure their reliability. Crop N model testing exercises usually compare measured and simulated values for aboveground crop N and inorganic soil N levels, and datasets of this nature are commonly available. Phosphorus (P) modelling in cropping systems is less advanced than N modelling, mostly due to complexities in estimating P sorption on the soil matrix and limited knowledge of the effects of P deficiencies on crop development. P datasets suitable for testing crop model performance are also very limited.

For field-scale model testing and validation purposes, a range of historical datasets were scrutinized, after which three datasets were judged appropriate. These datasets were collected in the Netherlands (Groot and Verbene, 1991), Kenya (Probert and Okalebo, 1992) and South Africa (Schmidt, 1993), and were selected according to suitability, primarily based on the scale at which the data was collected and the variables involved. The Netherlands and South African datasets allowed the testing of N modelling subroutines exclusively, while the dataset from Kenya included both N and P.

Measured datasets at the point- to field-scales for N and P export from cropping systems, especially with regard to leaching losses, are mostly confined to lysimeter and small plot studies. For this reason, a trial was initiated to collect data on vertical N and P movement in a soil profile. A drainage lysimeter located at the University of Pretoria Experimental Farm was utilized for this purpose. Briefly, swiss chard was grown under irrigation and soil water nitrate (NO_3) and P concentrations were monitored at various depths using ceramic suction cups (active sampler) and wetting front detectors (passive sampler). Using two types of samplers would potentially provide measurements of both the mobile and immobile soil water solute concentrations, and it was hypothesized that these mobile and immobile concentrations could be simulated using SWB-Sci – a mechanistic, generic crop model originally developed as a real time irrigation scheduling tool (Annandale et al., 1999a).. Depths at which monitoring was done were 15, 30, 45 and 60 cm. Any water draining from the bottom of the lysimeter was measured and analysed for NO_3^- and P concentrations.

In SWB-Sci, a layered, cascading approach is used to simulate the soil water balance. The approach developed by Corwin et al. (1991) to simulate incomplete solute mixing/bypass flow in soil water has been incorporated. The approach utilizes a mobility coefficient (γ) which represents the fraction of the liquid phase that is subject to piston-type displacement, with the fraction 1-γ therefore representing the liquid phase that is bypassed. The mobility coefficient is a parameter that must be specified by the user and will be related to soil texture. To the best of our knowledge, the approach developed by Corwin et al. (1991) or any similar approach has not been tested against measured NO_3 concentrations from active and passive samplers.

As hypothesized, suction cup concentrations aligned closely with immobile soil water concentrations, while wetting front detector concentrations aligned closely with mobile soil water NO_3 concentrations. Soil P concentrations were adequately monitored using wetting front detectors, but were often slightly over-estimated by the model. This indicates that these samplers clearly sample different soil water phases as hypothesized; and that the use of the Corwin et al. (1991) approach incorporated in a straightforward cascading soil water balance model with a daily time-step, was effective in modelling the impacts of the mobile and immobile soil water components on solute transport. Furthermore, using ratios of wetting front detector to suction cup NO_3 concentrations served effectively to estimate a mobility coefficient.

A major implication of this is that measuring and modelling can be used together to improve estimates of NO_3-N leaching losses. In using such an approach, a mechanistic crop N and P model such as SWB-Sci is used together with data from wetting front detectors and suction cups to calibrate and test the model for a specific site. Under field conditions, drainage data is rarely available to calibrate a model, as was done in this Task. These results, however, indicate that suction cup and corresponding wetting front detector NO_3^- concentration data can be used to estimate specific drainage parameters for the soil, and if wetting front detector and suction cup NO_3 concentrations are well estimated by the model over time, then it can be assumed that drainage will also be accurately estimated. In addition, measured N concentrations together with water flux estimates obtained from a simple crop soil water balance model can also be used to estimate leaching. Suction cup concentrations can be used during ‘slow’ drainage events and wetting front detector concentrations can be used during ‘fast’ drainage events, as indicated by the model. Further work to analyse how the mobility coefficient is influenced by soil texture, wetting front strength and antecedent soil water content is recommended.

5.1.2 *Applied & Predictive Research*

Development of SWB-Sci, a field-scale nitrogen and phosphorus crop model

SWB-Sci is a mechanistic, generic crop model originally developed at the University Of Pretoria, South Africa, as a real time irrigation scheduling tool (Annandale et al., 1999a). The commercially available version is called SWB. Evapotranspiration is calculated according to the Penman-Monteith grass reference method as recommended by the Food and Agricultural Organization (FAO) (Smith et al., 1996). Extensive crop parameterization work had been done locally for SWB-Sci, and testing exercises had shown that the model can representatively simulate the soil-plant-atmosphere continuum (Jovanovic et al., 1999; Jovanovic and Annandale 2000; Jovanovic et al., 2002; Tesfamariam, 2004). The chemical equilibrium routine of Robbins (1991) had been included into SWB-Sci and it had been used extensively to study the feasibility of irrigating crops with gypsiferous mine water (Annandale et al. 1999b; Annandale et al., 2002).

As part of this Project, N and P subroutines have been included into the existing SWB-Sci model. The decision to include N and P into SWB-Sci, rather than “import” a candidate model from international sources, was made for several reasons. Further development of an existing in-house model that had been thoroughly tested in terms of soil water dynamics would ease the challenge of the crucial code modifications and complex calibrations required when customising the model for different cropping systems and for doing long-term simulations. The model also needed to be applied by the same research Team in a parallel project on the assessment of the sustainability of biosolid applications to croplands as a disposal strategy. It was furthermore felt that further development of an existing in-house model would ultimately accelerate the development of new capacity in NPS N and P pollution modelling in South Africa. Finally, this Team’s interest in wetting front detectors and suction cups required an in-house model for ongoing analysis of fine-scale processes involved in vertical solute movement, making SWB-Sci a suitable model for inclusion of N and P simulation capabilities.

Wherever practicable, algorithms from well-established existing models were used. N and P simulation approaches and algorithms in SWB-Sci are based largely on those used in CropSyst (Cropping Systems Simulation Model) (Stöckle et al., 2003) for N, and GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) (Muller and Gregory, 2003) for P. SWAT (Soil Water Assessment Tool) (Neitsch et al., 2002) and APSIM (Agricultural Production Systems Simulator) (Keating et al., 2003) were also used, but to a more limited extent. CropSyst is described as a multi-year, multi-crop, daily time-step crop simulation model. GLEAMS is based on CREAMS (Chemicals, Runoff and Erosion From Agricultural Management Systems), which was developed by the U.S. Department of Agriculture's Research Service to evaluate agricultural NPS pollution from field-scale catchment areas (Knisel, 1980). CropSyst is written in the Visual Basic programming language, GLEAMS in the Fortran programming language, while SWB is written in Delphi.

As CropSyst uses a different approach to estimate yield, several modifications were required to adapt the N uptake and stress effect algorithms for SWB-Sci. Briefly, in CropSyst, yield is calculated as a fraction of total dry matter production using a harvest index, and N stress effects on yield are only calculated at harvest. In SWB-Sci, after flowering has commenced, a daily harvestable dry matter increment is calculated. Crop N available for translocation to the grain, as well as a yield stress factor based on a supply:demand ratio, is therefore calculated daily in SWB-Sci until physiological maturity. Modified algorithms to simulate crop P demand and uptake, P stress effects on crop growth were also required to ensure compatibility within the SWB-Sci approach to estimating crop growth. The N and P processes that have now been included into SWB-Sci are listed in **Table 5.1**.

Table 5.1: Nitrogen and phosphorus processes simulated in SWB-Sci

NITROGEN	PHOSPHORUS
Organic matter mineralization	Organic matter mineralization
Immobilization	Immobilization
Nitrification	P soil adsorption
Denitrification	Inorganic/organic N fertilization
Ammonia volatilization	Banded P fertilization
Symbiotic N fixation	Crop uptake, P stress effects
Inorganic/organic N fertilization	Soluble P runoff losses
NH_4^+ soil adsorption	Inorganic P leaching losses
Crop uptake, N stress effects	
Soluble N runoff losses	
Inorganic N leaching losses	

Parameterization of SWB-Sci for N and P simulations

Soil parameters required to simulate N are sand and clay percentage, organic matter percentage, soil pH (H_2O), cation exchange capacity, and soil layer nitrate and ammonium levels. In addition, the simulation of P requires a soil test P input; and depending on whether the soil is grouped as calcareous, slightly weathered or highly weathered, base saturation or calcium carbonate content is required.

The lack of detailed parameterization data is a common limitation to model application (Sharpley, 2007). During the model development phase it became clear that obtaining P initialization soil parameters for South African soils was highly challenging. Two fundamental difficulties were identified: the first was categorizing South African soils as slightly weathered, highly weathered or calcareous according to guidelines which were more appropriate for soils classified according to the USDA taxonomic system. The second was the estimation of soil labile P using soil P tests popularly used in South Africa, but which were not included in the original work done by Sharpley et al. (1984). These issues were addressed in this Project and specific guidelines were developed to assist model users in the parameterization of South African soils. The guidelines were published as a scientific paper – Van der Laan et al., 2009 – and enable catchment-scale modellers to utilize land type maps, which are available for the whole of South Africa at a scale of 1:250 000 (and the accompanying Memoirs), to parameterize models.

Model testing and validation
During model testing with the N datasets from the Netherlands and South Africa, the model was judged to simulate N dynamics in cropping systems more than adequately. The newly introduced approach to simulate the effect of N stress on yield on a daily basis following flowering, as opposed to simulating the effect of N stress on the harvest index as used in CropSyst, proved to be effective. **Figure 5.1** depicts the satisfactory correspondences of simulated with observed values for a lysimeter trial for total aboveground dry matter, N and P, conducted as part of this Project.

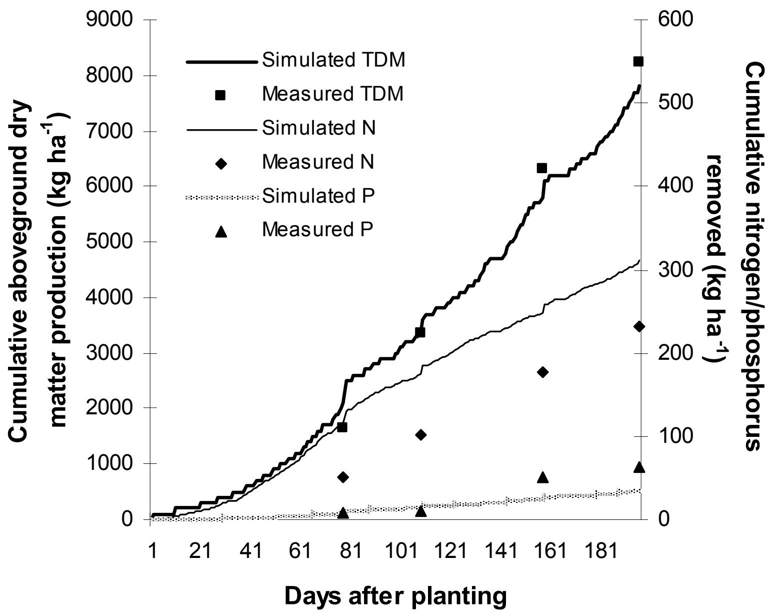

Figure 5.1: Cumulative aboveground dry matter (TDM) production (primary y-axis), and N and P removal (secondary y-axis) over the growth season

As also observed by De Willigen (1991), aboveground N variables were more accurately simulated than belowground N variables. Simulated changes in soil inorganic N levels and trends over the growth season often corresponded to measured values. In simulating organic matter in soils, the model requires that users input the size of the different fractions making up the soil organic matter (SOM), including the 'microbial biomass', 'active labile SOM', 'active meta-stable SOM' and 'passive SOM', at different soil depths. These fractions influence mineralization and immobilization rates significantly; therefore, it is important that they are accurately represented for the particular soils being simulated. Freshly mineralized inorganic N is clearly an important contribution to crop available N, and development of a simple laboratory procedure to assist users to obtain these values could be highly beneficial.

Using a dryland maize dataset collected in Kenya, the model simulated aboveground dry matter production (TDM), yield, leaf area index (LAI), profile water content, aboveground N and P mass, and grain N and P mass with varying levels of accuracy. Unfortunately, soil N and P levels had not been measured in this trial, which made testing and comparison of measured and simulated values more difficult. Except for aboveground P mass, agreement between measured and simulated values was almost always better for the first growth season than for the second growth season. Exact reasons for poorer performance by the model during the second season are not immediately clear. There could have been something that happened in the field when transitioning from the one season to the next that is not adequately captured in the simulations, or some of the newly developed algorithms still need further improvement; therefore, further testing and refinement of these newly included algorithms is recommended.

5.1.3 *Management Support Research*

Long-term simulations with SWB-Sci were used to compare leaching losses from a dryland and an irrigated cropping system and to assess the effectiveness of different pollution mitigation/control measures for the irrigated system. Data from a field trial conducted in the Free State, South Africa, was used to initialize and calibrate the SWB-Sci model. The objective was firstly to compare N leaching from a dryland and irrigated cropping system. Secondly, the effectiveness of strategies to reduce deep drainage and associated N leaching for a specific cropping system were analysed. The pollution mitigation/control measures tested were: (i) a split fertiliser N application strategy, (ii) a ‘room for rain’ irrigation strategy, (iii) a crop rotation strategy, and (iv) a crop rotation strategy incorporating a ‘room for rain’ irrigation strategy. Finally, the robustness and suitability of SWB-Sci to investigate and identify field-scale N leaching mitigation measures was assessed.

Annually, N leaching was estimated to be 433% higher for the irrigated system compared to the dryland system. Counter-intuitively, the split-application practice led to a higher mean annual N leaching being estimated by the model than for the standard single application irrigation system over the simulation period. The ‘room for rain’ irrigation strategy was able to reduce N leaching by 11%, while the crop rotation strategy was even more effective, with estimated N leaching being reduced by 42%. Employing a crop rotation practice as well as a ‘room for rain’ irrigation strategy simultaneously reduced N leaching most effectively (58%). Nevertheless, this strategy still led to estimates of N leaching 182% above that estimated for the dryland system. Results from this study demonstrate that pollution mitigation/control measures can significantly reduce N leaching from irrigated agriculture, but not to levels observed for dryland production. Future work considering unit leached per unit yield will assist in further improving comparisons of dryland and irrigated agriculture with regards to pollution potential.

While the mitigation measures tested here represent some of the more popular approaches, these are not exclusive, with many other options possible. The most appropriate mitigation measures will always be site-specific. For example, on a shallower soil profile, a split N fertiliser application strategy may have been more effective in reducing N leaching than estimated for the soil used in this study. Irrigating two crops a year may not always be possible, and water availability and irrigation system design will be a major factor in determining what mitigation measures can be implemented. When assessing different mitigation measures, it should also be ensured that the model is adequately describing the important processes. A possible shortcoming in SWB-Sci in assessing mitigation measures could arise from limitations in the simulation of active and passive soil N uptake and luxury N uptake, and how this influences the performance of a specific mitigation measure, for example applying split applications of N fertiliser or N as part of a fertigation strategy. In such cases of uncertainty, field trials and monitoring become important to validate model results and improve process simulation approaches.

In conclusion, long-term point-/field-scale modelling shows excellent potential in identifying the most suitable site-specific mitigation measures to reduce leaching losses, but the capability of the model to accurately describe the important processes must be considered.

5.2 Team: Pesticide Modelling (Jovanovic et al., 2012)

5.2.1 *Fundamental Process and Field Research*

As part of the Pesticides Task, a nested, experimental catchment, depicted in **Figure 5.2**, was established in the Western Cape, South Africa, located in the mid-reaches of the Berg River, in the vicinity of the town of Riebeek-West, on the farm, Goedertrou. It was deemed that the characteristics of the Goedertrou small-scale catchment (SSC) would be suitable to establish an experimental station for monitoring pollutant flux processes at point-, field- and small-catchment-scales.

Figure 5.2: Experimental scheme in the Goedertrou small-scale-catchment on a Google Earth map

The point- and field-scales were represented by standard Wischmeier runoff plots (22.3 m x 2 m) established in the field at the beginning of the experiment in 2005. The small-catchment-scale was represented by the farm dam collecting water from the Goedertrou SSC, which was approximately 20 ha in size. The common crop rotation in the area is one season of dryland wheat followed by 2 years of fallow land to regenerate soil fertility and for re-growth of previously cultivated grasses (e.g. wheat or medic grass) for pasture. Due to the lithological characteristics, steep slopes (about 10%) and shallow soils (about 0.5 m) overlying almost impermeable Malmesbury shale, overland flow and throughflow were thought to be the dominant water balance processes. The associated pollutant fluxes of relevance occurred via overland flow and at the interface between the soil and consolidated shale, where temporary groundwater accumulates. It was surmised that the agricultural activities carried out during the course of this project had little effect on deeper groundwater.

In order to describe water and pollutant fluxes in the system, the following data were collected from 2005 to 2009 (unless specified otherwise):

- Hourly and daily weather data collected with an automatic weather station (rainfall, solar radiation, air temperature, relative humidity and wind speed; the weather station was supplied by Mike Cotton Systems, Cape Town).
- Yield of wheat in 2005 and 2008, as well as re-growth of grasses on fallow land in 2006 and 2007.
- Hourly volumetric soil water contents measured with Echo sensors connected to a data logger (Decagon Devices Inc.), at two depths in the soil profile and at two positions along hillslopes. The purpose of the electronic measurement of soil water content was to identify the build-up of temporary water tables in winter, and to quantify throughflow using water retention curves and saturated hydraulic conductivities. This subsurface flow was an important component of the water balance due to soil and geological characteristics of the area. Spot-checks of soil water content were done with the gravimetric method in 2005 to test the manufacturer’s calibration of the Echo sensors.
- Overland flow measured at 10 minutes intervals during runoff events from the Wischmeier runoff plots (from 2005 to 2008). The runoff plots were set up to collect a portion of the overland flow volume in tanks for laboratory analyses of pollutants.
- Pesticide concentrations in soil and runoff water were measured approximately monthly: Methomex (active ingredient methomyl) and Folicur (active ingredient tebuconazole) were applied in 2005 and MCPA was applied in 2008. Pesticide concentrations were measured in dam water approximately monthly.
- Nutrient (N and P) concentrations in the soil root zone and runoff water were measured approximately monthly in 2005; nutrient (N and P) concentrations in the soil and plant material were measured once in 2006.
- Measurements of sediments mobilized from the runoff plots (total sediment concentrations and sediment size distribution with a Saturn Digisizer LASER particle size analyzer, Micromeritics Instrument Corporation) from 2006 to 2008, following each runoff event that filled collection tanks with water from the Wischmeier runoff plots.
- Water level in the dam collecting water from the Goedertrou SSC was measured hourly with an Eijkelkamp Diver during 2008.
- Geological maps, 20 m Digital Elevation Map and soil maps.

Summary of primary observation findings:

- The Goedertrou SSC is in a semi-arid area and during this Project annual rainfall varied between 232 mm in 2006 and 456 mm in 2008. Low intensity rainfall occurs mainly in winter (from May until October).
- Wheat grain yield was between 2 Ton/ha (in 2005) and 3 Ton/ha (in 2008). Total biomass production from fallow land was between 2 and 2.7 Ton/ha (in 2006).
- Volumetric soil water content varied depending mainly on seasonal rainfall and vegetation. South-oriented, clayey soil retained more water than North-oriented, lighter-textured soil. Soil water contents exhibited high spatial variability depending on soil physical properties.
- Overland flow on the runoff plots was between 4% and 19% of annual rainfall, depending on vegetation, soil type, slope and orientation.
- Different land uses caused different volumes of overland flow. Bare soil and less densely planted soil produced more overland flow. Different soil properties, slopes and antecedent

moisture conditions also caused different volumes of runoff. In general, more overland flow occurred from uncultivated land, and from land oriented towards South, with steep slope and clayey soil.

- The maximum flux of pesticides measured in runoff water was 1.38 g/ha for tebuconazole (rainfall/runoff event 2 days after application in 2005). No rainfall occurred after application of methomyl in 2005. Both methomyl and tebuconazole, applied towards the end of the 2005 wheat season (end of rainy winter), degraded rapidly in situ and did not have a significant impact on surface waters in the absence of rainfall. Half-lives in dam water were 23.6 days for tebuconazole and 4.4 days for methomyl.
- No detectable traces of MCPA in dam water were observed after application of this herbicide in the first week of July 2008 and subsequent rains that occurred during the 2008 winter season.
- Based on overland flow volumes and NO_3 concentrations measured at the Wischmeier runoff plots, it was calculated that between 0.24 and 3.65 kg/ha of NO_3 were mobilized via overland flow during 2005. NO_3 and PO_4 concentrations in runoff water collected at the runoff plots varied widely depending mainly on the timing of fertiliser application and rainfall/runoff distribution.
- The temporal patterns of nutrient concentrations in both soils and surface water followed mainly fertiliser applications. Very low concentrations of NO_2 were generally measured. A time lag was observed between the application of fertiliser and increase in concentrations of NO_3 in runoff water, as nutrients were washed out by erratic events. The concentrations of NO_3 and PO_4 in dam water were in the range of those measured in runoff water.
- Concentrations of sediments in runoff water were between 0 and 22.0 g/ℓ (2.6 g/ℓ on average), depending on rainfall distribution and intensity, slope and vegetation. Total seasonal sediment mobilization ranged between 0.02 and 0.85 Tonne/ha/a (0.26 Tonne/ha/a on average).
- High concentrations of sediments in runoff water were generally measured when small runoff events occurred (low rainfall amounts and/or intensity). With high rainfall and runoff volumes, sediment concentrations were generally low due to dilution effects. In terms of total sediment load, however, more eroded material was mobilized from the runoff plots during heavy rainfall and runoff events. The bulk of mobilized particles had diameters in the range between 5 and 15 µm (silt range), depending on the soil texture (source of mobilized sediments) and slope (gravity force for transport), and regardless of rainfall and overland flow volumes. The expected sediment particle size distribution in the catchment can be used in conjunction with sorption data to estimate transport of sorbed contaminants, e.g. nutrients and pesticides.
- Water levels in the dam at Goedertrou varied seasonally and responded within hours of rainfall events.

5.2.2 *Applied & Predictive Research*

One of the first activities carried out in the Pesticide Task was to identify priority processes and variables for pesticides in order to improve/augment existing models/methods applicable to different scales. The Task included a description of priority processes, their mechanisms, relevant factors and variables, quantification (measurement and prediction) as well as mitigation measures. This led to the identification of the following priority processes concerning water and pesticide fluxes:

<u>Overland flow and pesticide transport</u>: Along with leaching, pesticide transport via overland flow is the most direct process involved in the contamination of water resources. In runoff water, pesticides are transported as both solutes and adsorbed on suspended particles and organic matter. Pesticide transport via overland flow depends mainly on environmental conditions (in particular rainfall), application rates, physico-chemical properties of pesticides, type of vegetation and management practices. Mitigation/control measures include vegetated buffer areas, inter-row vegetated filter strips

and agricultural ditches. Other mitigation/control measures to pesticide transport via overland flow are conservation tillage, in particular by incorporating pesticides in the soil, constructed wetlands and water soluble polymers, which prevent erosion and enhance infiltration.

Vertical water and pesticide fluxes: Along with transport via overland flow, leaching is the most direct process involved in the pesticide contamination of water resources. Pesticide movement in the soil profile occurs by infiltration, convection, mechanical dispersion due to variations in velocity through pores of different size, and diffusion. Although the principles of water and pesticide fluxes in the intermediate (vadose) zone are those typical for porous media, the rate of pesticide transfer and transformation in sub-soils is often unknown and difficult to establish. The sub-soil zone generally differs from the overlying soil root zone because of lack of organic matter, different temperatures, microbial activity, water content, texture and structure. Mitigation/control measures to reduce pesticide leaching are generally considered to be appropriate pesticide application (rate and timing relative to rainfall) and irrigation scheduling.

Preferential flow: Preferential flow pathways allow rapid travel of pesticides in porous media. Shorter travel times due to preferential flow reduce diffusion of pesticides into soil aggregates. Therefore, less attenuation (through sorption, decay and volatilization) occurs before pesticides reach the groundwater. Dual-permeability models are generally used to predict transport of pesticides in preferential pathways and the soil matrix.

Throughflow and pesticide transport: Contamination of surface waters can also occur via throughflow in layered soils, where movement of water and pesticides may occur on sloping impermeable layers. Pesticide transported through interflow can be intercepted by the root zone of vegetative filter strips.

Pesticide plant uptake: The main processes to be considered here are plant uptake of pesticides from the soil via the transpiration stream, diffusive exchange with air, stomatal uptake from air of micropollutants sorbed to fine particles, metabolism, plant death and harvest. Plant uptake of pesticides depends mainly on plant species, seed characteristics and growth stage, intended use (selectivity), soil characteristics such as pH, temperature, clay fraction, moisture content, organic matter content, the type of pesticide, the pesticide formulation and properties (sorption and degradation), the method of application and mode of action, pesticide concentration and contact time. Mitigation/control measures commonly considered are the use of appropriate chemicals (selectivity), rates and timing of application.

Volatilization is the process where solutes move from the medium where they are dissolved into the atmosphere. Volatilization may occur from soil and plant surfaces, from water surfaces as well as from the soil matrix. Volatilization can cause atmospheric transport, downwind off-target movement, deposition and contamination of the environment.

Sorption is the attraction of pesticide molecules to soil particle surfaces. This process influences the pesticide fluxes by retarding pesticide migration. Pesticide sorption occurs mostly on organic matter and, to a limited extent, on soil mineral particles. It depends mainly on pesticide properties, solution properties (e.g. presence of ortho-phosphates, ionic strength and dominant ions), soil-chemical contact time (aging), soil properties (e.g. soil particle sizes determining the surface area and sorption sites, type and nature of clay, soil pH and temperature, and especially soil organic carbon and humic substances) and soil management practices (e.g. tillage). Sorption can be artificially modified through organic amendments used to enrich soils of low organic matter contents.

Pesticide persistence (degradation, decay) is a highly complex process. Degradation may occur through microbial activity, depending mainly on pH, temperature and moisture (biodegradation), through photochemical reactions due to absorption of electromagnetic energy by a pollutant (photodecomposition), or chemically by reacting with oxygen (oxidation) or water (hydrolysis). Degradation can be artificially modified through amendments used to enhance microbial activity (e.g. delivery of oxygen, nutrients etc.) or shallow incorporation into the soil (e.g. reduction of photodecomposition).

As volatilization, sorption and degradation are inherent properties of specific pesticide species, mitigation/control measures for these processes can generally be considered to be the choice of chemicals, quantities and timing of application.

Numerous process models available internationally are capable to simulate the priority processes identified in this project. The following models that were screened in this Task satisfied most of the criteria: FIRST, GENEEC, HYDRUS_2D (including the code originating from SWMS_2D), PELMO, PESTAN, PRZM, SWAP, SWAT and VS2DT. A demonstration of pesticide redistribution in the soil profile on a hillslope and pesticide degradation was carried out with the HYDRUS_2D model for methomyl and tebuconazole, using intensive monitoring data collected in the Goedertrou SSC in 2005 (point-scale simulations).

The application of process models to predictions of pesticide impacts on water resources presents, however, serious challenges (Boesten, 1999; Meinhardt, 2003). Some of the challenges are the complexity of the soil-plant-atmosphere system, large extent and intensity of input data required, large number of chemicals available on the market with specific properties, lack of knowledge on pesticide behaviour and toxicity as well as spatial and temporal uncertainties. Also, it is generally infeasible and prohibitively expensive to establish intensive monitoring experiments for a large number of pesticides, factors affecting their fate and behaviour, as well as mitigation/management measures. An alternative to process-based models is the use of expert systems, which are interactive computer programs that include quantitative informational databases and qualitative knowledge, experience and judgment gained over many years of work and research. They can be used as support to both decision- and policy-making. For this purpose, the output of the expert system is often expressed in the form of simple environmental performance indicators or indexes. It was therefore decided that an expert system for modelling the fate of pesticides at field-scale be developed.

The development of expert systems and the compilation of guidelines for the use of pesticides and their environmental impacts are not novelties. Expert systems and environmental impact indicators for pesticides that were published include EXPRES (Crowe and Mutch, 1992), LIMPACT (Neumann et al., 2003), Ipest (Van der Wef and Zimmer, 1998), EIQ (Kovach et al., 1994) and Environmental Yardstick (Reus and Leendertse, 2000).

Some gaps identified in both dedicated pesticide process models and expert systems/environmental indicators were:

- Environmental costs are seldom considered because of the difficulties in assigning costs to indirect (external) economic values (e.g. ecological functions, opportunity costs etc.), in particular when data and resources are limited.
- Mitigation/management practices are seldom considered, i.e. both process models and environmental indicators are not sensitive to mitigation measures (e.g. wetlands and buffer strips, anti-erosion contours etc.).
- Both process models and environmental indicators are generally applicable to a specific scale (field- or catchment-scale).

In this Task, we addressed these gaps through the development of an expert system (guidelines) to assess the mobility of pesticides and their potential for accumulating in water resources.

The Pesticide Environmental IndeX (PestEX) is an Excel-based calculator that accounts for the main factors affecting the contamination of surface- and groundwater, namely pesticide drift, position of application in relation to streams and groundwater, general slope of the area, dominant flow direction (vertical or horizontal due to the presence of impervious layers in soils), tillage practices, soil hydraulic properties (saturated hydraulic conductivity), irrigation practices/rainfall distribution (affecting overland flow and deep percolation), pesticide properties (volatilization, sorption and degradation), pesticide application and sensitivity of the receiving water resource. The novelty of the approach is that the factors were combined based on their occurrence at different scales. Mitigation/control measures (wetlands/buffer strips and anti-erosion contours) are also considered to be factors in the calculation of environmental mobility of pesticides. Each factor is scored (rating x weighting) to produce a combined environmental score. Pesticide application is used to calculate an economic score corresponding to pollution abatement costs. Fuzzy logic normalization of the factors allows comparison and minimization of environmental and pollution abatement costs.

Being written in Excel, PestEX is easy to use and interactive. An Excel worksheet is dedicated to the input and calculation of each influential factor and it can be accessed by clicking on the relevant command button in the Main Menu (main worksheet). Any factor can be disabled by clicking on tick-boxes. The programme makes extensive use of pop-up comments to facilitate the user in operating as well as selecting the inputs. Links to databases, reviews and references are available within the programme. The graphs are interactive and they automatically show input data and ratings for each factor. Nearly-linear relationships described with fuzzy logic could be substituted with non-linear functions, should these be available. For example, the relationship between yield reduction and pesticide application cannot always be approximated with a straight line. Similarly, abatement costs increase as more pollution is abated. Additional factors can be easily incorporated in the program; for example, solubility of chemicals or effects on air quality, providing some information is available on the behaviour of chemicals in the environment and depending on the specific objectives to be achieved.

It should be borne in mind that the PestEX index is not meant to give a direct measure of field- or catchment processes. However, some of the factors considered may be more relevant to the field-scale and others to the catchment-scale. The non-relevant factors for a particular application can be disabled. It should also be noted that PestEX gives a normalized environmental index based on several input variables. Absolute values of contamination will depend on the total quantities of pesticide applied and the dilution capacity of the receiving water body. These can be obtained through measurements, and/or predicted with transfer functions and process models.

5.2.3 *Management Support Research*

It is envisaged that potential users of PestEX might be the scientific community, farmers, pesticide consultants and regulatory authorities. The primary applications envisaged are comparative analyses of mobility and exposure potential (say, between two or more pesticides or factors), and sensitivity analyses (say, effects of changing one or a combination of factors). Furthermore, applications can be the comparison of environmental and pollution abatement costs of different chemicals for regulatory or marketing purposes, sensitivity analyses to assess the effects of different mitigation/management measures (e.g. size of wetlands to be constructed), the minimization of costs by changing mitigation/management practices, etc. For all purposes, a calibration and validation of the model is recommended by adjusting the weighting of each factor, and comparing the output to measured data. The sensitivity of PestEX should be calibrated and tested at different sites and for different pesticides.

A description of the procedure used, the Excel-based calculation of the PestEX indicators, and an example of an application comparing methomyl and tebuconazole applied at Goedertrou in 2005 are included in Jovanovic et al. (2012).

5.3 Team: Catchment-Scale Modelling (Lorentz et al., 2012)

5.3.1 *Fundamental Process and Field Research*

For this Task, a nested, experimental catchment, the Mkabela catchment, was established in a sugar cane growing area near Wartburg, KwaZulu-Natal, South Africa (**Figure 5.3),** in order to examine the migration processes of pollutants from the field-scale to the catchment-scale, through surface and subsurface pathways to receiving waterways, as well as through the controls and links affecting the pollutant fate. The catchment monitoring was designed to enable detailed observations in a small headwater sub-catchment, with nested sampling points at progressively increasing contributing areas. In this way the relative influence of a pollutant source in the catchment, illustrated by a square in **Figure 5.3**, could be assessed at the outlet of the catchment (large circle) through an understanding of local processes, terrestrial connectivity (dotted line) and in-stream controls. Conversely, this understanding is also required to assess the effectiveness of on-site remediation management/pollution control measures for reducing the relative impact on the catchment-scale pollutant load.

The catchment study served a number of purposes as follows:

- To observe water, sediment and nutrient transport processes from the field- to catchment-scale and thereby guide model use and development,
- To integrate the respective Teams, working at different scales and with different water quality variables, in a common endeavour at a field site and
- To allow for the calibration and testing of models against observed data.

Overland, subsurface and in-stream water, nutrient and sediment processes were observed in the experimental catchment, while intermittent discharge measurements were made and water sampling taken at the series of nested stations illustrated in **Figure 5.4.** Comprehensive soil and land use surveys were completed in the catchment and the main stream network was surveyed and described. The land use in the catchment comprised primarily sugar cane, but with scattered areas of forestry, vegetables, maize, pastures, wetlands and farm dams, as shown in **Figure 5.4**.

Observations of water, nutrient and sediment movement were made at scales ranging from point to catchment. Point- and field-scale observations, respectively, were undertaken in six soil water dynamics profiles and two Wischmeier overland flow runoff plots (22.3 m x 2 m). Overland flow was recorded automatically at the runoff plots and an integrated sample was collected for nutrient and sediment analysis. Soil water tension was logged at quarter hour intervals in the profiles and cores were extracted during selected wet and dry periods for soil nutrient analysis. Further field-scale observations were undertaken at an automatic flow measuring flume in a waterway. Flow-rated samples were automatically extracted and analysed for nutrients and sediments. A similar flume was positioned at the small-catchment outlet, where accumulated water, nutrient and sediment fluxes from a number of sugar cane compartments were observed.

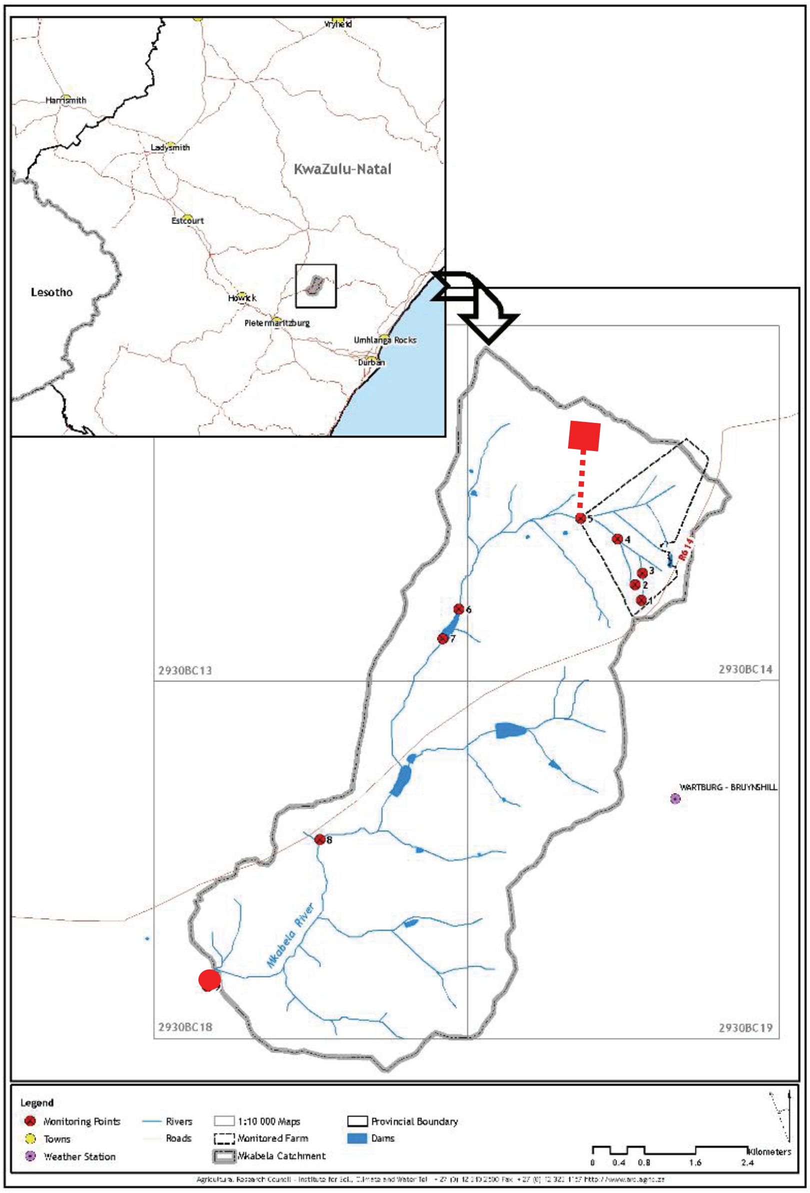

Figure 5.3: **The Mkabela catchment near Wartburg showing the research catchment in the headwaters, nested sampling positions and an illustrative source (square) with terrestrial flow pathway connection (dotted line) to stream network.**

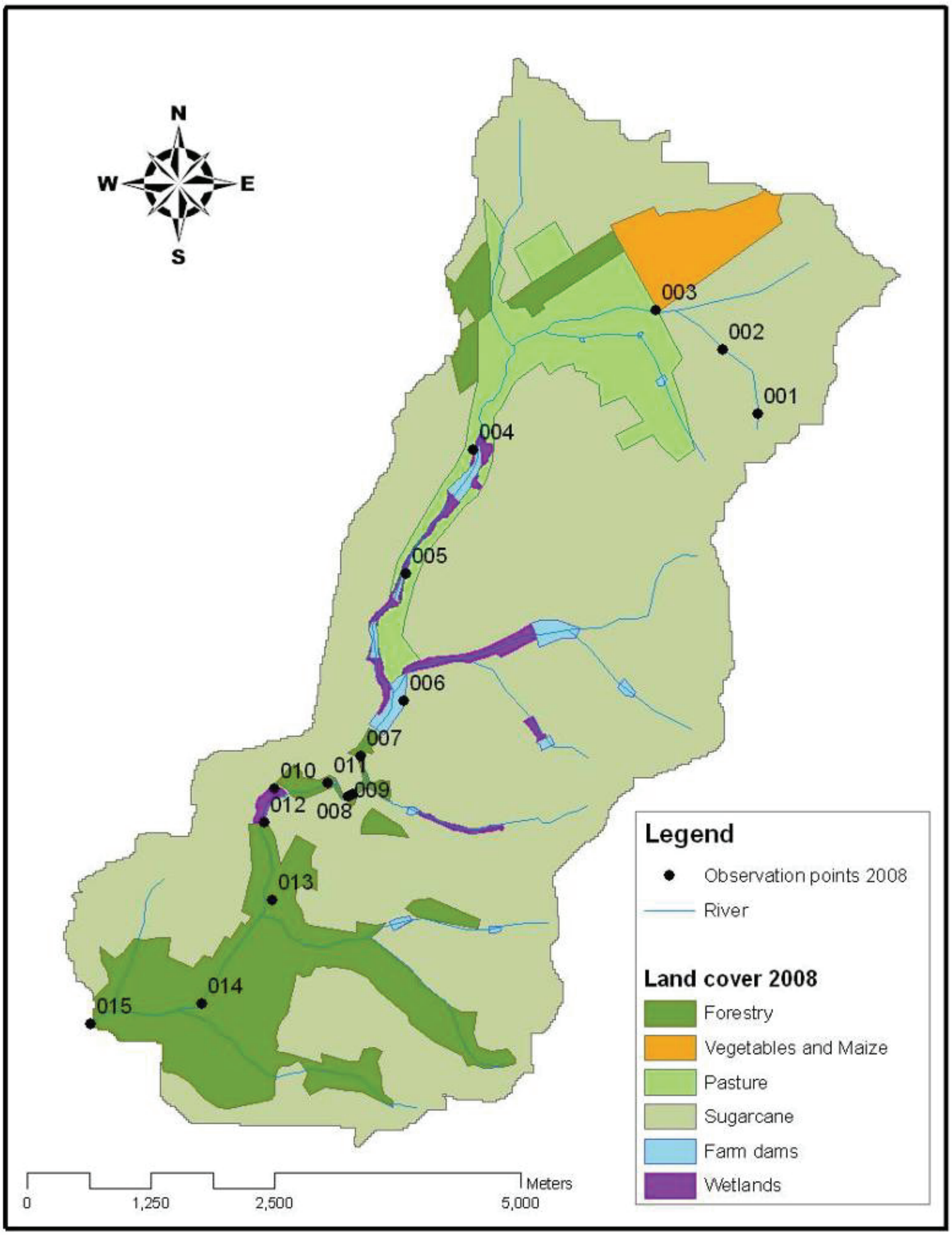

Figure 5.4: Land Use in the Mkabela Catchment

Catchment-scale observations comprised periodic sampling for nutrients and sediments at selected stations representing increasing catchment areas (**Figure 5.3** and **Figure 5.4**). Observation of water, nutrient and sediment dynamics at the various scales began in November 2005 and continued until 2010. Specific periods of observation, however, were selected to illustrate the general responses at field- to catchment-scales.

Summary of primary observation findings:

- Soil water tensions responded to rainfall events of more than 30 mm to a depth of 400 mm below surface in the soil profile. This reflects the rapid delivery of water to the subsurface and the dominant role of preferential flow in the delivery of water between point- and field-scales at this site.
- The yield of suspended solids and nutrients from overland flow was dependant on the growth stage of the sugar cane. Significant increases in runoff and nutrient yield were observed at the larger field- and small-catchment-scales compared with the smaller field-scale, indicating a predominance of subsurface discharge from the sugar cane land use. Particularly noticeable was the increase in P:sediment load ratio between the smaller and larger field-scales. This suggests a contribution of P through subsurface discharge, which is likely to be associated with organic P applied in the form of fertiliser.
- The proportion of load increase between the upstream Flume 1 and downstream Flume 2 is higher than the incremental area between the two flumes, indicating a higher response to runoff and mass loading in the lower, flatter slopes of the small catchment draining to Flume 2. This also reflects the accumulation of upslope subsurface contributions.
- Yields of suspended solids and nutrients were highly dependant on “controls” (small impoundments) in the water flow path, including road-crossings, farm dams and wetland areas. Occasional high flow events yielded increased loading from farm dams when these were disturbed by the high rate of change in water volume. Concentrations of all NPS–P species drop significantly after the road-crossing sampling station. However, these increase downstream after the dam outflow station, reflecting increasing loading with increasing contributing area downstream of the “controls”.
- Suspended solids and nutrient concentrations generally increased during a runoff event, reflecting the available source of sediments and nutrients.
- Groundwater responses appear to be affected by event loadings, confirming the rapid delivery of nutrients to the vadose zone profile.

5.3.2 *Integrative Tools Research: Catchment-Scale Models*

Two catchment-scale process-based modelling systems were implemented and tested during this Task. These were the RSA-developed ACRU Model, customised during this Project to incorporate nutrient-crop dynamics, and the internationally-established SWAT Model, applied in its most current form. These models are fully referenced in the paragraphs below.

5.3.2.1 *THE ACRU-NPS MODEL*

Outline of Modelling Approach

ACRU is a deterministic agrohydrological model – developed in South Africa – based on the SCS runoff generation algorithm (Schulze, 1995) that simulates daily discharge and peak runoff from daily rainfall. Sediment yield per unit area, from a land unit is based on the Modified Universal Soil Loss equation (Lorentz and Schulze, 1995), in which the energy for sediment entrainment and transport is derived from the event discharge volume and peak flow rate. Empirical soil erodibility, vegetative cover, slope and practice factors are used to determine the sediment yield at a catchment scale from the event intensity and discharge energy.

Inclusion of nutrient mass balance algorithms in *ACRU* enabled simulation of:

- N and P losses in surface runoff, sediment, and leaching
- N and P cycling in the soil-water-plant-animal system
- N and P mass balances in the watershed system.

The resultant "*ACRU-NPS*" includes rainfall, irrigation, fertilisers, plants, and animal wastes as potential nutrient sources and represents management impacts on N and P transformations and transport. Since the GLEAMS model (Knisel and Davis, 1999) included most of these capabilities in its current version, it was used as a guide in the development of *ACRU-NPS*.

ACRU-NPS was programmed using object-oriented tools. New component objects were added to *ACRU* to represent a plant residue layer, a soil surface layer and plant matter removed from the system being modelled. Process objects were developed to model soil temperature, snowfall, snowmelt, ammonification, nitrification, N plant uptake and fixation, volatilisation, denitrification, N adsorption and extraction, ammonium partitioning coefficient, immobilization, P mineralisation, P plant uptake, P adsorption and extraction, labile P partitioning coefficient, harvest, tillage, surface transport, evaporation transport, and subsurface transport. Process objects also were developed to handle nutrient inputs and to initialise nutrients. Numerous data objects were created to facilitate data input and output, and to hold nutrient status information.

Nitrogen Processes
The Nitrogen Cycle comprises N in one of several forms: Organic N, Ammonium, Ammonia, Nitrite, Nitrate, and N_2 (gas). The transformation of N into these different forms happens via the following processes, which are all included in the model: ammonification, immobilization, denitrification, nitrification, fixation, uptake, and volatilization are simulated, with specific options for fertiliser and animal waste application (as Organic N), crop N uptake and runoff, and leaching/sediment losses. There are ten types of Nitrogen represented in GLEAMS and *ACRU-NPS*: Fresh organic N, plant N, assimilated N, fertiliser, Nitrate, Ammonia, N_2 (gas), active soil N, stable soil N, and organic N from animal wastes.

<u>Mineralization</u>
Mineralization occurs from active soil N, fresh organic N, and organic N from animal wastes in two stages: a first-order ammonification process and then a zero-order nitrification process. The active mineralizable N pool is defined using carbon to nitrogen (C: N) ratios from 12-25. The long-term stable N pool (no mineralization occurs) has a C: N ratio less than 12. There is also an N flux between the two pools, which is governed by their relative sizes.

Ammonification of organic nitrogen from animal waste on the surface is added to a soluble surface ammonium pool in the surface soil layer. Nitrification of the soluble surface ammonium is assumed to occur on the soil surface and is then added to a soluble nitrate pool. Both the soluble nitrate pool and the soluble surface ammonium pool are accumulated and immobilized onto residue until rain or tillage occurs. Rain or tillage events cause them to return to the surface layer where they are again added to the nitrate and ammonium pools.

<u>Immobilization</u>
Using the C: N ratio method described in the previous paragraph, immobilization is defined as the range of C: N greater than 25 at which microbes assimilate N onto the residues from sources such as soil nitrate and ammonia. Immobilization ceases when the C: N ratio reaches approximately 25. If the amounts of nitrate and ammonia available are less than the immobilization estimate, the decay rate is

adjusted to let only 95% of the NO_3-N and NH_4-N in layer 1 be immobilized, and the fresh residue in each layer is then reduced. Surface residue immobilization is simulated in the same manner, with the exception that for surface residues, the ammonium and nitrate pools in the soil layer of interest are combined with the separate surface pools produced by surface mineralization processes.

Denitrification

Soil nitrate can be denitrified to N_2 (gas) by anaerobic bacteria when soil water content is greater than the field capacity. This is an especially important process in humid, high water-table environments. Denitrification in *ACRU-NPS* (and GLEAMS) is first-order, as a function of organic carbon, with a rate constant and soil water content and temperature effects. Fresh organic residues, organic C in animal waste, and organic C in the potential mineralizable N pool participate in the reaction. Denitrification begins at 10% above field capacity, and increases to a maximum of unity at saturation.

Denitrification is subtracted from soil NO_3 for each layer on each simulated day, and occurs in the upper soil layers on days with rainfall or irrigation (when percolation from the root zone may not occur), and in the lower soil layers (when percolation may occur for an extended period due to perched water tables).

N losses in runoff, sediment, and percolation

The movements of chemicals with runoff are dependent on the chemical type and the soil characteristics. Incomplete extraction of chemicals in the surface soil layer into runoff will occur. The general equations for determining chemical concentrations available for runoff and infiltration in the upper soil layer are the same for nitrate, ammonia, phosphorus, and pesticides.

Ammonia is partially adsorbed, thus the adsorbed portions are dependent on erosion and sediment losses, and is a function of sediment yield, solid concentration, and enrichment ratios. In deeper soil, less ammonium and nitrate are available for percolation because of runoff losses. Percolation of nitrate and ammonia in deeper soil layers is determined as a function of their concentrations in the surface soil layer, which is calculated by their concentration relative to the dry weight of the soil. The percolation component is then found as a ratio of total available mass and total concentration of available nitrogen.

N losses to uptake, evaporation, fixation

Nitrogen uptake is calculated by the concentration of biomass-N expressed as a power function of total dry matter.

All crops differ in their ammonia and nitrate uptake capabilities, however, the model assumes that uptake is equal to the relative mass of each N-species in the soil layer being considered for transpiration processes. N concentration in plant biomass is a function of empirical coefficients, Leaf Area Index (LAI), total dry matter, and N dry matter. Ammonia and nitrate uptake are found from a calculation of the concentration of the chemical in the water, and the transpiration calculated for each layer of root growth. Total uptake is found by summing over the number of transpiration layers. An overabundance of nitrate and ammonia is assumed to not result in a flush of uptake. If soil N is greater than a threshold value, leguminous plants will take N from the soil. If soil N is less than that value, these plants will fix N_2 from the atmosphere. Nitrogen demand for a leguminous plant is calculated, then the ammonia and nitrate concentrations in the solution phase are summed in layers where transpiration occurs.

Ammonia and nitrate are moved upward in the soil one computational layer above the one at which evaporation occurs. It is assumed that movement up one layer is caused by water flux, and then by vapor flux in additional layers. Ammonia is not volatilized from the surface. The equations governing nitrate and ammonia evaporation from a layer result in an enrichment of these species in the surface 1 cm of soil, for subsequent runoff and percolation processes.

Rainfall and Fertiliser N

Nitrogen can also be instantaneously added to the system via fertiliser and rainfall, the latter of which contains both ammonia and nitrate. These processes are simplified by assuming that all rainfall N is as nitrate. Separate nitrate and ammonia pools are maintained, allowing nitrate and ammonia fertilisers to be considered separately. Fertiliser and animal waste can be applied on the surface, incorporated, injected, or fertigated. Application of inorganic fertiliser on the soil surface is assumed to mix with the appropriate species upon tillage or rainfall.

Ammonia Volatilization

Ammonia losses to volatilization are high from surface-applied animal waste, but drastically reduced when the waste is incorporated post-application. Volatilization is also dependent on the storage and handling of the waste, and the environment where the waste is applied. In ACRU-NP, volatilization is considered as a non-point source related to air temperature, calculated daily for one week after application or until rainfall or tillage occurs. It is assumed that volatilization occurs only for surface applied solid, slurry, and liquid animal waste. Liquid waste or immediate incorporation of solid and slurry wastes are assumed to volatilize for six hours. After rainfall, remaining ammonia in the waste is added to the surface soil layer's soluble ammonia pool, where it is assumed that it cannot be volatilized.

Phosphorus Processes

The GLEAMS phosphorus component incorporated into *ACRU-NPS* was largely derived from that in the EPIC model (Sharpley and Williams, 1990). The main modification was adding the mineralization of organic phosphorus in animal waste. Many of the governing processes in the phosphorus component mirror that of the nitrogen component. The description below is largely derived from the GLEAMS Manual by Knisel and Davis (1999).

The Phosphorus Cycle comprises phosphorus in one of several forms: organic P, labile P, and inorganic P. Transformation of P into these different forms happens through different processes: mineralization, immobilization, fixation, and adsorption. There are three soil P pools: mineralizable organic humus, active mineral and long term stable mineral. Analogous to the N component, the P pools are defined by their respective C: P ratios. Fresh organic P generally has a C: P ratio greater than 200, while mineralizible organic humus P pool has a range from 125-200. The active mineral P pool aids in immobilization of labile P by sorption. The sorption of phosphorus is a function of soil characteristics.

Mineralization

Mineralization of phosphorus is simulated as a single-step first-order process, following the same general procedure as nitrogen. Seventy-five % of the mineralization from fresh organic P is added to the labile pool, while 25% is added to the organic humus pool. Phosphorus in the surface residue is mineralized to soluble P in the same manner as fresh organic P. The ratio of active and stable soil N pools is used to partition soil organic humus P into the mineralization fraction. The flow between the active and stable mineral P pools is defined as a function of soil water, temperature, labile P, the P sorption coefficient, and active mineral P. When this flow is positive, the daily amount is added to the stable soil pool from the stable mineral pool. When negative, the reverse is true. At equilibrium, the stable mineral P pool is assumed to be four times the active mineral pool.

Analogous to the nitrogen component, the mineralization rate of phosphorus in animal waste is calculated from the decomposition rate constant, the organic P in the animal waste, soil water, and temperature factors. Seventy-five % of the P mineralization from animal waste is added to the labile pool, and 25% is added to organic humus pool.

Immobilization

Immobilization of plant available labile P occurs when C: P of crop residues is greater than 200. The general governing processes are the same as for N, with the exception that there is only one source of P to immobilize. Immobilization can be limited by either P or N, and immobilized P is subtracted from the labile pool and added to the fresh organic pool. Surface immobilization is calculated in the same method as that for N, and subtracted from labile P in the top soil later and added to P in the surface residue.

P losses in runoff, sediment, and percolation

Phosphorus adsorption and partitioning follows the same processes as that for ammonia, as they are both adsorbed to the soil clay fraction. The model assumes that the partitioning coefficient for phosphorus is related only to the soil clay content.

Phosphorus concentration in the top soil layer that can go to percolation or runoff is calculated from the concentration of labile P based upon the dry weight of the soil times an exponential function analogous to ammonium. This, and the partition and extraction coefficients, determines the concentration of P in water. The concentration of P in water then enables the calculation of P in runoff, and in the sediment associated labile P. The percolated mass of P is calculated using the soil dry weight P concentration. Total P sediment losses are finally found using sediment P from animal waste, active and stable mineral P, and sediment humus P.

P losses to uptake and evaporation

Phosphorus demand and subsequent uptake data of N:P ratios are available for 78 different crop simulations in the model, although the average N:P ratio is about 7:1. The phosphorus demand is determined as the difference between the total dry matter P on successive days. Labile P uptake is estimated for each layer in which transpiration occurs, and total uptake is a sum over all transpired layers. Adjusted P demand is subtracted from the labile P pool for each layer; however, growth is not constrained for P deficiency, like it is in the N component. Phosphorus moves upward with evaporation in the same way as N, with the same assumptions. Movement by evaporation in the non-top soil layers is also the same as for the N component.

Fertiliser P

Inorganic P fertiliser is assumed to be instantaneously available plant available labile P. If it is surface applied fertiliser, the surface mass is added to the soluble P pool, and into the surface layer with rain or irrigation. The solubility of different forms of P based fertilisers are not considered.

Crop Growth and Harvest Yield

Crop growth and harvest yield are functions of reductions in potential yield due to stresses caused by reduced water or nitrogen availability to the plant. The greater of the two stresses is applied to a daily increment in Leaf Area Index, which is used in the subsequent time-step to generate transpiration and growth increment. A new algorithm for stress recovery, based on a logarithmic trend towards the optimum state, has been found necessary and has been coded and extensively tested. **Figure 5.5** outlines the linkages between stress and crop yield in *ACRU-NPS*.

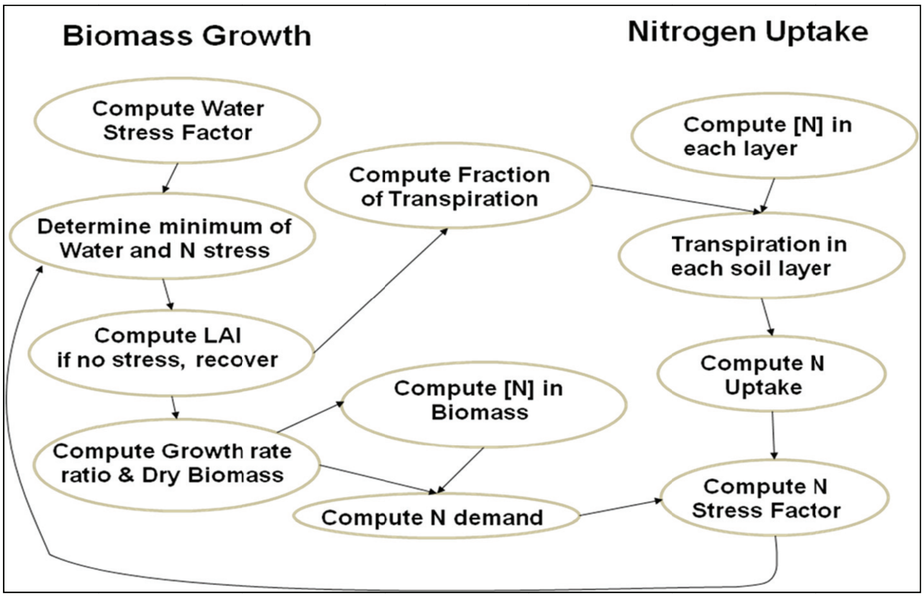

Figure 5.5: Water and nitrogen stress and crop growth processes

NPS-Pollution Controls

Controls to the migration of sediments and nutrients have been introduced to the output of the land-based mass balance. An Excel model was developed to route pollution loads through the on-farm and in-channel control measures and the in-stream controls such as wetlands and dams in the river channels in the catchment to determine losses of pollutants in the system. These are based primarily on algorithms in the SWAT model.

Outcomes of Model Testing

The following outcomes from the model development and testing against observed loads have been documented.

- Guidelines for estimating certain parameters was developed using point-scale knowledge of nutrient dynamics and guiding soil mapping techniques. Close interaction with the SWB-Sci development Team played a major part in the successful compilation of the guidelines.
- Simulated NO_3 loads were similar to those observed, while simulated P loads were lower than observed.
- Subsurface delivery of water and possibly P was poorly simulated, which could be the reason for the low simulated P concentrations.
- Simulated sediment loads were higher than observed during the wet season and were likely excessively high for dry season, extreme rainfall events. The sensitivity of the soil erodibility to simulated antecedent water content might be the reason for over-simulation of sediment yields during wet periods.
- Simulation of the large-scale catchment demonstrated pollution load reductions due to in-stream, wetland and reservoir processes.

5.3.2.2 THE SWAT MODEL

Outline of Modelling Approach

The Soil and Water Assessment Tool (SWAT) model was selected to identify source areas and key processes of transport of NPS pollutants from field to stream at a large catchment scale. SWAT is a catchment-scale model that was developed at the US Department of Agriculture (USDA) Agricultural Research Service (ARS) to predict the impact of land management practices on water, sediment, and agricultural chemical yields on complex landscapes with varying soils, land use, and management conditions over long periods of time (Arnold et al., 1998). The intention was not to improve and augment SWAT as was done with *ACRU-NPS*; rather, the intention was to provide a comparative catchment-scale alternative to *ACRU-NPS*.

In SWAT, surface runoff volume is computed using the SCS curve number method which is empirically based and relates runoff potential to land use and soil characteristics (USDA Soil Conservation Service, 1972). Peak runoff rate is estimated with a modification of the Rational Method; where runoff rate is a function of daily surface runoff volume and a proportion of rainfall occurring until all of the catchment is contributing to flow at the outlet. The latter duration is estimated using Manning's Formula, considering both overland and channel flow. Sediment yield is computed with the Modified Universal Soil Loss Equation (MUSLE). In addition, loading functions estimate the daily organic N/P runoff loss based on the concentration of organic N/P in the top soil layer, the sediment yield, and the enrichment ratio.

Once the loadings of water, sediment and nutrients have been determined for all specified sub-catchments, SWAT routes the loadings through the stream network of the catchment. Flow is routed through the channel using a variable storage coefficient method, including transmission losses leaching through the streambed and return flow or base flow originating from groundwater. Sediment is routed by means of stream power theory, where the maximum mass of sediment that can be transported from a reach segment is a function of the peak channel velocity. Nutrients are routed through the channel using equations from QUAL2E (Brown and Barnwell, 1987), whereby the model tracks nutrients dissolved in the stream and nutrients adsorbed to the sediment.

The crop growth and yield component of SWAT is a simplified version of the EPIC plant growth model. Phenological plant development is based on daily accumulated heat units. Potential biomass is based on a method that converts energy to biomass using photo-active radiation and Leave Area Index parameters. Plant growth can be inhibited by temperature, water, nitrogen or phosphorus stress and vice versa. Finally, the crop yield is partitioned from the total biomass and is reported as dry weight. The integrative character of the fate-of-pollutant chemical and physical processes is further illustrated in the validation and comparison of results in Lorentz et al (2012).

Application of the MUSLE equation requires that site-specific vegetation parameters must be accurately derived to assure successful model performance. Unfortunately, many of the required land cover parameters could not be obtained directly from existing data for the Mkabela catchment. Given a lack of data on the actual crop rotation systems and timing of agricultural operations, phenological plant development was based on daily accumulated heat units. As a result, research rather focused on improving simulations by revising or incorporating only the most significant catchment components in the model for which appropriate input data existed.

Figure 5.4 depicts the distribution of land use for the simulation period of 1 July 2004 to 30 June 2008. Although SWAT was configured to simulate all the nested sub-catchments in the catchment, the number of observed events and sub-catchments/outlets in which both streamflow and pollutant concentrations could be measured were minimal (five events at the two flumes located in the upper sub-catchments). Thus, verification of the simulated loads at the larger scale (main catchment outlet) was not possible. Nonetheless, five successive simulation runs were used to calibrate the model and improve simulated results against the observed values by revising or incorporating important model components and parameter settings in an incremental fashion. These improvements included the following:

- Division of the initial soil components into smaller soil units using ARC-ISCW terrain unit data, and up to three layers incorporated into each soil component
- The inclusion of multiple hydrological response units (HRUs) to account for soil and cover diversity. (HRUs are portions of a sub-catchment that possess unique land-use/soil attributes).
- Incorporation of nine outlets that represent nodes/outlets at the exit from farm dams
- Incorporation of important hydrological structures, i.e. wetlands
- Modification of the default SCS Curve Number (CN) of sugarcane
- Delineation of sub-catchments into hydrological response units to capture the diversity of land use
- Adjustment of Manning's roughness coefficient (n) for hydrological response units and channels
- Incorporation of important management practices, i.e. tillage operations, nutrient applications, irrigation scheduling, and harvesting operations.

Outcomes of Model testing

Compared to observed values, simulated results for sediment concentration/loads obtained at the end of the above incremental calibration improved on average by 30%. SWAT successfully tracked most of the peak flow events that occurred during the year, although the peaks were usually over-predicted (by approximately 100%). In contrast, the majority of the low-flow periods were slightly under-predicted (by approximately 30%). Exactly the opposite holds for sediment concentration. Sediment concentrations for peak flow events were usually under-predicted (by approximately 400%), whereas the sediment concentration for the majority of the low-flow periods were slightly over-predicted (by approximately 200%).

A possible cause of the above outcomes could be unrepresentative trap efficiencies of the nine farms dams as simulated by SWAT in the Mkabela catchment. For example, small dams (e.g. 0.1 ha surface area) seem to have similar trap efficiencies to large farm dams (e.g. 10 ha surface area). Trap efficiencies of farm dams and their influence on NPS pollutants in the Mkabela catchment needs further investigation. The addition of 9 farm dams (instead of one) in the Mkabela catchment caused simulated flow rates to decrease on average by 18%, whereas sediment yields decreased by 89%.

In comparison with *ACRU-NPS*, the SWAT-simulated annual average pollution loadings in the Mkabela catchment were low. Primary causes of these discrepancies are likely to be different model representations of site-specific processes of overland versus subsurface discharge and nutrient flux. SWAT seems to incorporate adequately the physics of important hydrological structures, such as wetlands, farm dams and channel roughness. Furthermore, the GIS-interfaced model of SWAT (AVSWATX) was efficiently configured to include all the nested sub-catchments in the large catchment. The examination of loads at multiple scales in the large catchment revealed the effect of controls such as wetlands, riparian areas and farm dams on the progress of pollutants downstream.

5.3.3 *Management Support Research*

5.3.3.1 THE ACRU-NPS MODEL

Evaluation of the economic impacts of NPS pollution in agriculture must necessarily compare the benefits of specific land use practices on crop yield against the costs of deteriorated water quality.

The water quality impact may be assessed at the outlet of a farm unit/source area or at some position in the stream network downstream of multiple source contributions. The prediction of water quality impacts immediately downstream of a source can be used to evaluate load reductions due to remediation at each source, while predictions in the stream network can be used to determine the relative contribution from each source and, in so doing, to direct remedial measures and assess their net effects.

For this purpose *ACRU-NPS* was modified to include:

- Algorithms to simulate nutrient and sediment production from land segments for various land uses
- A crop growth algorithm in which the crop yield is influenced by water and nitrogen stress
- Algorithms to simulate nutrient and sediment fate at controls and buffers in the stream network, which also included provision for farm dams, wetlands and riparian buffer strips

With these modifications completed, a series of scenarios were analysed, based on the catchment configuration and observations made in the Mkabela catchment (described in Section 5.3.1) and a 50-year daily rainfall sequence. For the purpose of the scenario modelling, the catchment was divided into land segments based on the dominant land use, as well as on the in-stream and riparian network controls and buffers. **Figure 5.4** presents the land use distribution across the catchment. **Figure 5.6** depicts the catchment as a simplified network for scenario-modelling purposes.

The scenarios comprised:

- *Base case:* current land use (including contours);
- *No contours:* current land use, but no contours used in the sugar cane segments;
- *All sugar:* all land uses set as sugar cane;
- *Irrigation:* current land use, but with deficit irrigation applied to the sugar cane;
- *No buffers:* Base scenario with on-farm controls (farm dams and buffers) removed.

All these scenarios were run with a series of fertiliser applications, comprising current fertilization practice (Base), twice (high), half (low-1/2) and a quarter (low-1/4) of the Base fertiliser applications and finally, no fertiliser (zero) application.

The resulting simulated sediment and nutrient loadings into and out of the significant in-stream controls – the three large wetlands and the two large dams – were analysed comparatively for all these scenarios, as were sugar cane yields. Selected graphical illustrations of these comparative results follow in the sections below:

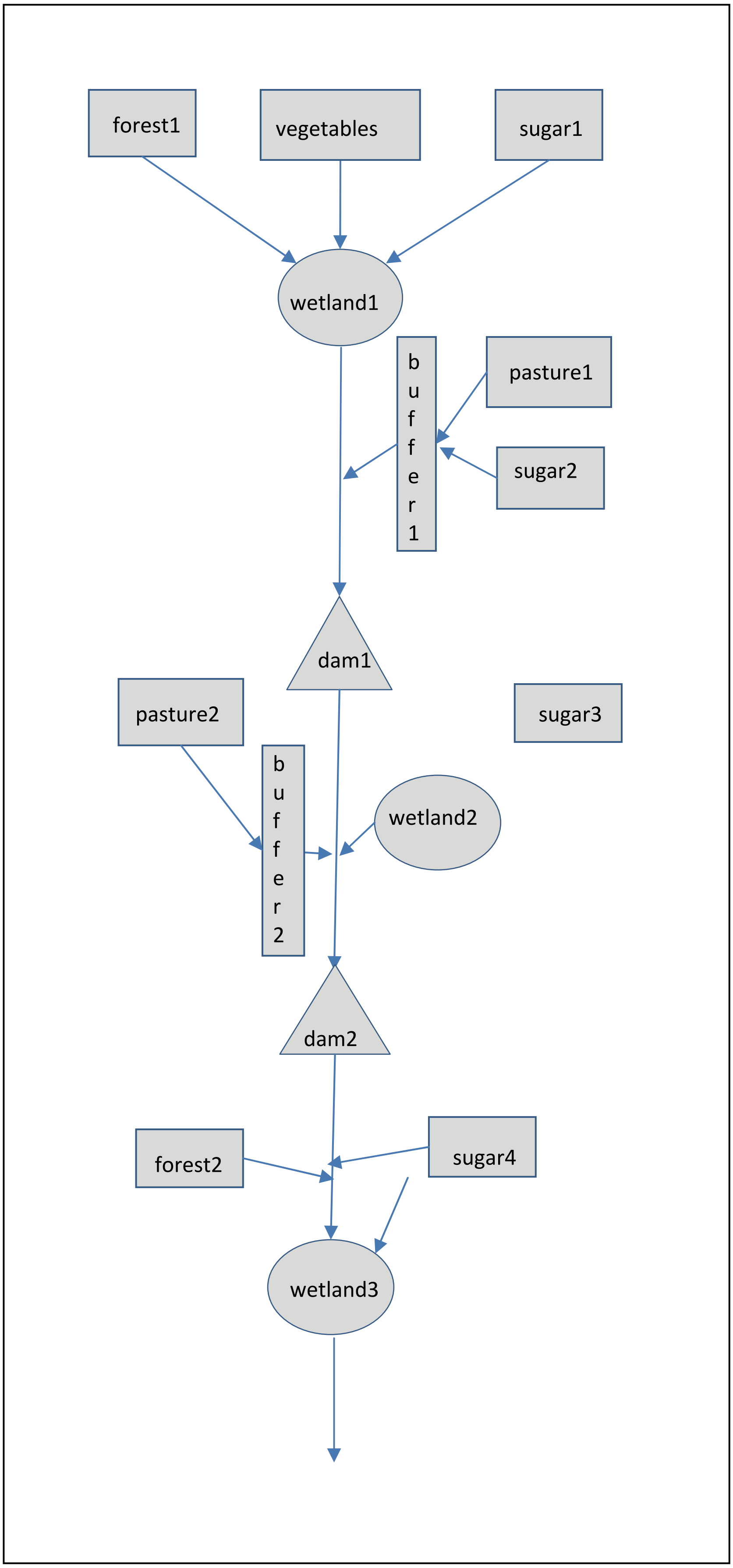

Figure 5.6: Mkabela Catchment as a Simplified Network for Scenario Modelling Purposes

Sugar Cane Yields

A 50-year rainfall record was used to simulate sugar cane crop yields and pollutant loadings for each scenario. The cropping period was assumed to be 18 months. The maximum potential yield was set at 75t/ha.

Figure 5.7 shows that the Base fertiliser application crop yields vary between 66t/ha and 34t/ha over the 50 year period. There is a marginal improvement in crop yield with the Double application rate and systematic, but small, decreases in yield with lower fertiliser application rates. Without fertiliser application, the crop yields are significantly lower than those from the Quarter application rate. However, there are two occasions when the crop yield without fertiliser exceeds the fertilized yields (1955 and 1957). This apparently occurs during these dry years due to the preservation of available water from a previous year's very low crop yield without fertiliser.

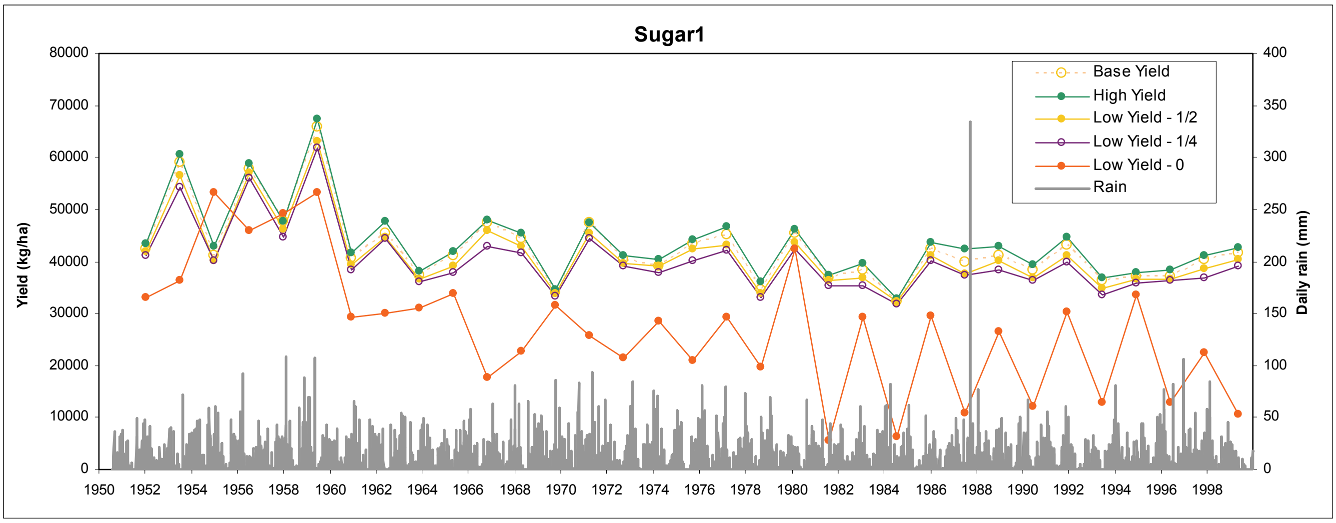

Figure 5.7: Sugar cane yields from Land Segment 1, for 50 year simulation

Nutrient and Sediment Loads

Daily runoff and mass loads of sediment, nitrogen and phosphorus have been simulated for the sugar cane catchment, LS1. These daily values have been accumulated for each 18-month cropping period so that catchment loadings can be compared to resultant crop yield.

Marginal reduction in runoff occurs with increasing fertiliser application rates as increases in plant water uptake are realised. Without fertiliser and with consequent reduction in plant water uptake, the runoff is generally higher than the fertilized scenarios.

N and P export varies significantly with varying fertiliser application **(Figure 5.8** and **Figure 5.9).** The consequences of over-fertilization are very clear in the large mass loads resulting from a doubling of the application rate, compared to halving the rate.

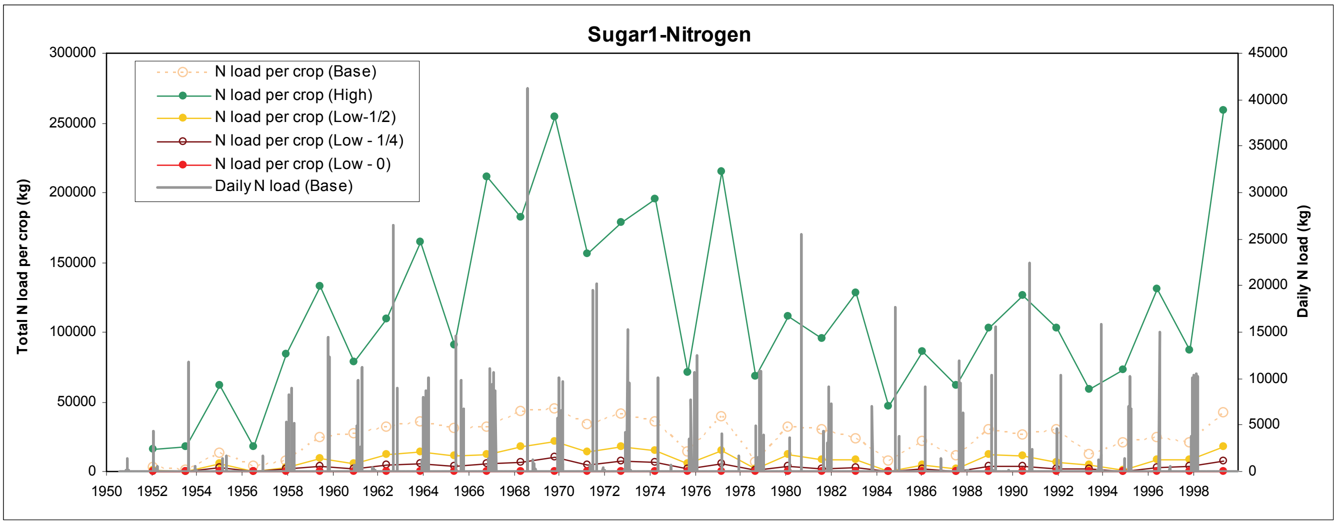

Figure 5.8: **Nitrogen loads from Sugar Cane Land Segment 1, for 50 year simulation, for all fertiliser application rates, Base and High to Low-0**

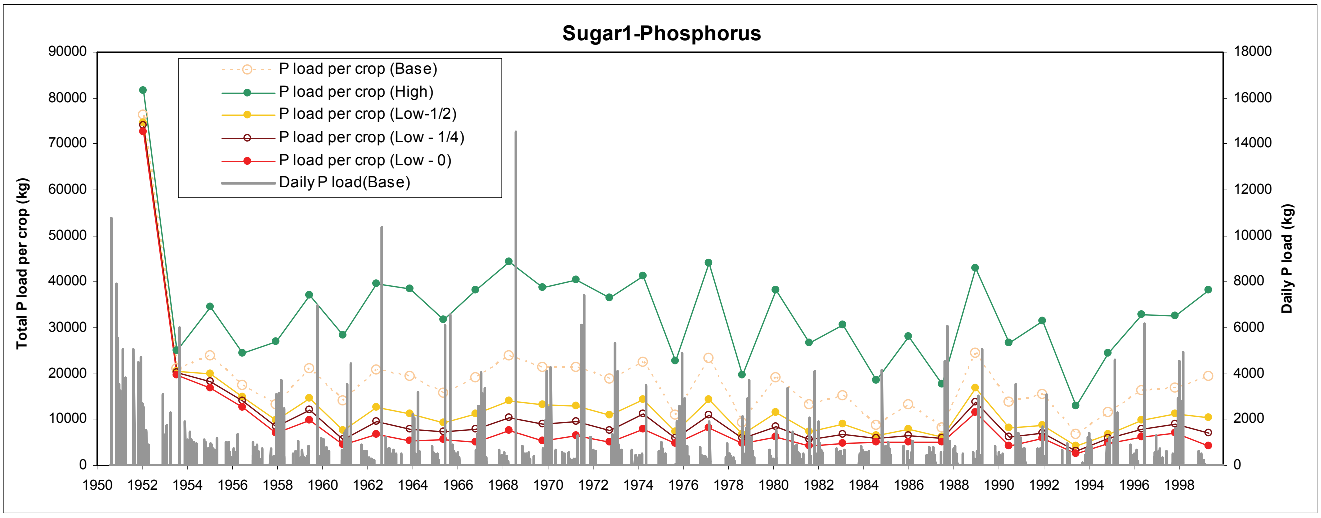

Figure 5.9: **Phosphorus loads from Sugar Cane Land Segment 1, for 50 year simulation, for all fertiliser application rates, Base and High to Low-0.**

Impacts of Physical Controls

The sugar cane yield, discharge, sediment and nutrient loads were routed through the river channel network and imbedded physical controls (see **Figure 5.6**). As an example of the outcomes, the resultant inputs and outputs at the Wetland 3 control at the outlet of the catchment are illustrated in **Figure 5.10.** The detailed findings are discussed in Sections 5.4.2.

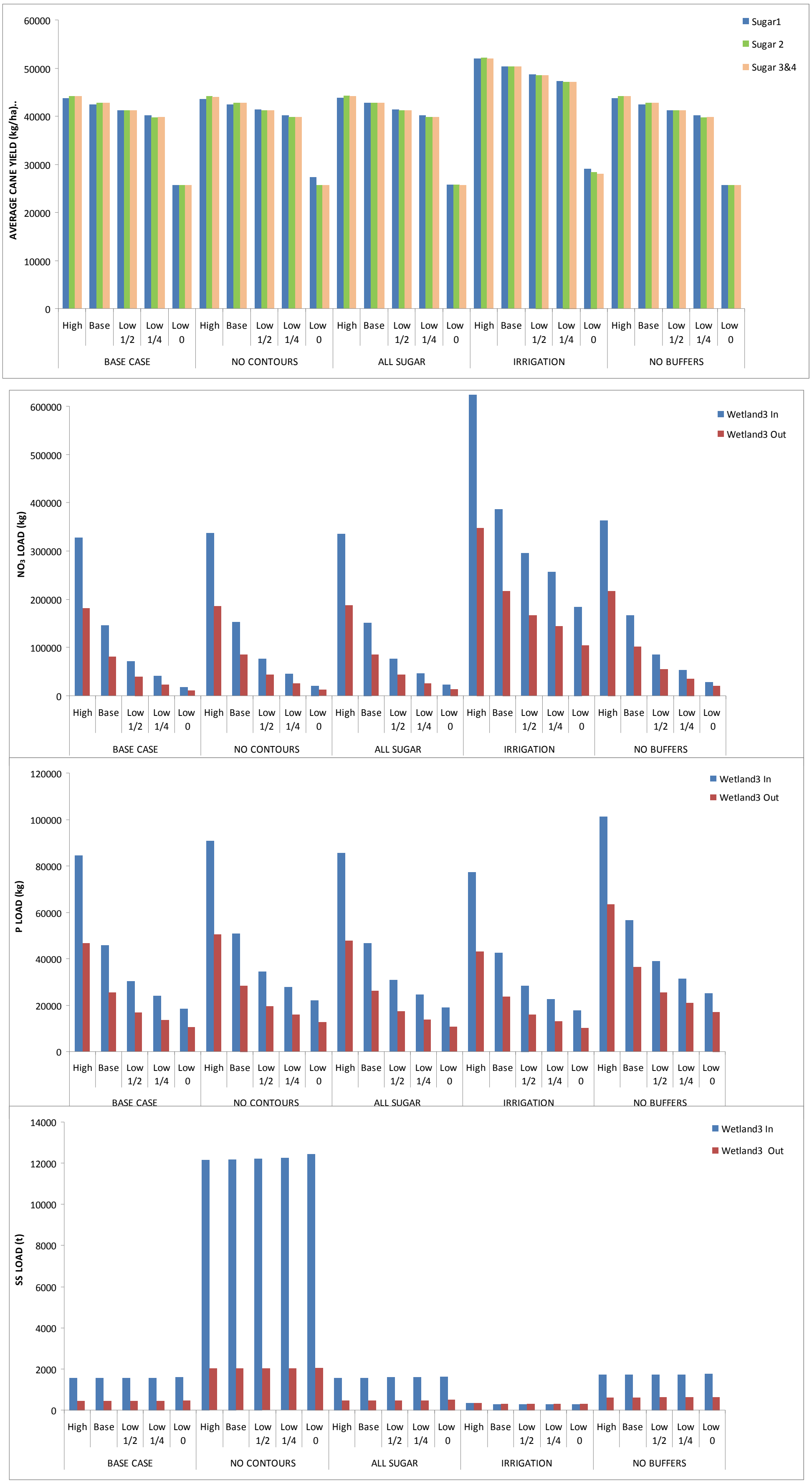

Figure 5.10: **Scenario annual averages for cane yield (top), NO3, P and sediment yields (bottom), into and out of Wetland 3**

5.3.3.2 THE SWAT MODEL

The relative impacts of eight alternative pollution management scenarios in terms of flow, sediment and nutrients at the outlet to the Mkabela catchment were examined using the SWAT model. The scenarios include the whole catchment under:

- S1 Sugarcane
- S2 Vegetables with soil being tilled
- S3 Vegetables with no till practices
- S4 Current cover and practices with zero nutrients added
- S5a Current cover and practices with 50 kg/ha mineral P and 100 Kg/ha mineral N applied
- S5b Current cover and practices with double nutrients applied
- S6 Current cover and practices, but excluding all wetlands
- S7 Current cover and practices with 1.5 m buffer strips surrounding cultivated fields.

Scenario Modelling Outcomes

The relative outcomes of the above eight scenarios, as simulated via SWAT, in terms of flow, sediment and nutrient loads are presented in **Table 5.2** as averages at the main catchment outlet.

Table 5.2: Scenario average outputs from Mkabela outlet for the simulation period Jan 2006 – Jun 2008

Scenario	**S1**	**S2**	**S3**	**S4**	**S5a**	**S5b**	**S6**	**S7**
Flow (m^3/s)	0.58	0.50	0.51	0.56	0.56	0.56	0.56	0.56
Sediment (mg/ℓ)	3.10	6.85	6.88	1.18	1.18	1.18	1.00	0.84
N (kg N/month)	35.3	302	276	92.0	747	1540	55.9	52.5
P (kg P/month)	0.19	33.6	30.4	0.99	1.87	3.54	0.63	0.22

Columns S2 and S3 indicate that sediment concentrations and both N and P loads at the catchment outlet will increase significantly when replacing other land use types with cabbage. Sediment output doubles when replacing other land use types with sugarcane (S1). Despite being a soil conserving crop, sugarcane is usually more prone to erosion than forestry plantations with good ground cover. Doubling the nutrients applied throughout the catchment (S5a and S5b), doubles N and P rates at the catchment outlet. Of all the scenarios, the buffer strip scenario (S7) produces the lowest output rates for sediment and the second lowest for N and P.

Also worth mentioning is the small difference between sediment, N and P outputs from cabbage with till (S2) and cabbage without till (S3). It is postulated that SWAT does not simulate till scenarios effectively, rather than the possibility that either of these scenarios does not exacerbate pollution in the catchment.

5.4 Team: Economics of Agricultural NPS Pollution Management (Matthews et al., 2012)

5.4.1 Integrative Tools Research

Arrow and Debreu (1954) proposed that uncertainty might be represented by a set of possible states of nature, which pioneered the state-contingent approach. State contingent theory suggests that a production function or pollution loading function exists for every state of nature. By implication every year (or every production cycle) would have a different function due to the effect of weather on production. The procedure negates the assumption of normally distributed errors imposed by the Just and Pope (1979) model. The procedures developed by Richardson et al. (2000) were combined with the state contingent production functions to model pollution risk by means of empirical distributions. The adopted modelling procedure was successfully integrated into a chance-constraint programming model to quantify economic environmental trade-offs of maintaining environmental targets at specified levels of assurance.

Use of chance-constraints requires prior knowledge of the distribution of pollution loads. Determining the specific form of the pollution load distribution is tedious since the same distribution may not hold for all situations due to the site-specific nature of agricultural NPS pollution (Qui, Prato and McCamley, 2001). To overcome the problem of specifying the distributional form, an upper partial moment (UPM) approach was developed based on the empirical distribution to enforce the chance-constraint. The UPM is based on the safety-first rule developed by Bunn (1999). The UPM model treats pollution loads as an empirical distribution and determines a target pollution level endogenously based on a user-specified environmental goal.

For this Task the state contingent approach was used to characterise pollution risk during crop production. Simulation results from both SWB-Sci and *ACRU-NPS* were used to fit crop production functions, irrigation-fertiliser response functions and pollution loading functions for each production cycle. The researchers specifically focused on developing procedures to synthesise the large body of output generated with the bio-physical models in the form of production functions and pollution loading functions taking cognisance of the heteroscedasticity and non-normality of the error terms. These functions were combined with economic data to estimate the margin above specified cost (MAS) for the farmers' production decisions.

To determine the economic-environmental trade-offs when maintaining environmental standards, two optimisation models were developed. The first model determines the optimal MAS with no constraint on pollution emissions. The results were used to determine the baseline pollution level, which is then constrained in the second model to determine environmental compliance according to user-specified goals or standards. Economic-environmental trade-off curves were developed by solving the compliance model for different levels of pollution abatement.

For the catchment-scale analyses, a node network specification was used to represent the layout of the catchment, and the linkages between the different land segments in the optimisation model. Every control (buffer, dam or wetland) within the catchment has two nodes associated with the control. The first node is associated with the point where pollutants enter the control while the second node is where the pollutants exit the control. Contribution factors were estimated to quantify the changes that occur as the pollutants move through a control. The use of contribution factors proved to be a powerful mechanism to link the pollution loads generated by land segments to the resulting pollution levels at any downstream point in the catchment.

5.4.2 Management Support Research

Scaled case study approach

Three case studies were undertaken to examine the trade-offs between economic benefits versus costs and water quality-related environmental benefits versus costs of agricultural pollution control measures at, firstly, field-scale and, secondly, farm-scale and, thirdly, catchment-scale.

For the field-scale analysis of economic-environmental trade-offs the SWB-Sci model was used to generate crop production-related information for irrigated late-monoculture maize at Glen Agricultural College in the Free State Province of South Africa. Production functions and pollution loading functions were developed for the following four scenarios:

- SCL_Single Sandy clay loam soil with a single fertilisation application

- SCL_Split Sandy clay loam soil with a split fertilisation application (two thirds at plant and a third seven weeks later
- SC_Single Sandy clay soil with a single fertilisation application
- SC_Split Sandy clay soil with a split fertilisation application (two thirds at plant and a third seven weeks later.

Optimal irrigation water use associated with the production of maize was also simulated. The model was set-up to allow for 40% depletion of plant available water before triggering irrigation. Irrigation water was then applied up to field capacity, thus the crop did not experience water stress during any stage of production. Production values were simulated for 18 production years between 1981 and 2000. Trade-off curves were developed for the two different soils (SCL and SC) and the two different management practices (split versus single application of fertilisers), respectively.

For the farm-scale analysis of economic-environmental trade-offs the SWB-Sci model was also used to generate crop production-related information for irrigated late-monoculture maize for the above 18 production years. The cultivatable soils mix of the farm was assumed to be 60 ha SCL and 30 ha SC. Only single fertiliser applications were specified.

The third case study was a demonstration of economic-environmental trade-offs at catchment-scale. The *ACRU-NPS* model was used to simulate the runoff and pollution from, as well as the crop production in, the Mkabela catchment (introduced in Section 5.3.1). The whole catchment consists of agricultural land, with sugar cane being the crop of choice and vegetable, pasture and forestry as alternative production systems. Production practices for sugar cane in the catchment were designed by SASRI (South African Sugar Cane Research Institute). SASRI production practices include field lay-out, agricultural practices used when growing the crop, contouring and waterway layout.

ACRU-NPS was set-up to simulate sediment and nutrient emissions from plantations, pastures, vegetables and sugar cane production in accordance with the simplified Mkabela River catchment set-up depicted in **Figure 5.5**. Production practices were varied on the sugar cane area only, while the rest of the areas were assumed to remain unchanged. Five alternative production practices for sugar cane were super-imposed on the model, all related to the fertilisation regime used. The fertiliser regime recommended by SASRI was taken to be the Base regime. Alternative fertiliser regimes were half of the recommended regime (half Base), a quarter of the regime (quarter Base), double the recommended regime (double Base) and zero fertiliser applications, respectively. The fertiliser applications consisted of organic and inorganic fertiliser. The inorganic fertiliser consisted of LAN 28% while the organic fertiliser was a sugar mill residue called Milo.

Production-related model outputs were generated for a period of 50 years with a production cycle of 18 months for sugar cane production, with and without field contours and buffers. Meta-models in the form of "contribution coefficients" were used to represent reductions in pollution loads as they move through the controls, i.e. buffers, dams and wetlands. The pollutant loads from the land segments, associated crop yields and contribution coefficients were used in a spatial network node optimisation model to determine economic-environmental trade-offs.

Field-scale economic environmental trade-off case

The optimised baseline characteristics for field-scale maize production are presented in **Table 5.3.**

Table 5.3: Optimised baseline for field-scale maize production on a SCL (sandy clay loam) and SC (sandy clay) soil for a single and split nitrogen application

		SCL		SC	
		Single	Split	Single	Split
Margin above specified cost (MAS) (maximised)	R/ha	3496	3203	3258	3021
Maize yield	ton/ha	6.3	6.0	6.1	5.9
Nitrogen fertiliser used	kg/ha	154	165	162	167
Irrigation water applied	mm	501	482	488	478
N Pollution output level	kg/ha/a	25.3	29.3	25.9	28.5
Area planted	ha	1	1	1	1

The trade-off curves developed for the four field-scale scenarios are depicted in **Figure 5.11** for a pollution output compliance assurance/probability of 90% and for incrementally more stringent environmental targets. For example, for the environmental target, Target_0, this means that during 90% of production years the N pollution output level is constrained to be less than the values specified in **Table 5.3.** The drastic drop shown in **Figure 5.11** in margin above specified costs (MAS) between the baseline and Target_0 may be interpreted as the "cost" of having to implement on-field controls/mitigations to limit pollution output exceedences of the "average" levels of **Table 5.3** to less than 10% of production years. The Target_10 to Target_50 slots in **Figure 5.11** represent environmental targets that are smaller (i.e. more stringent) than the baseline values by steps of 10%.

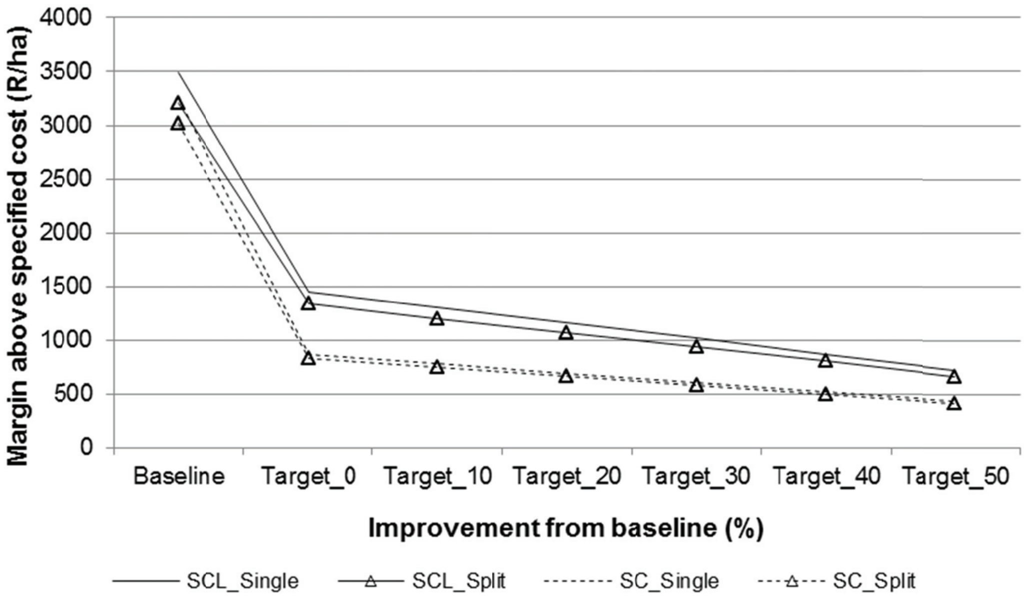

Figure 5.11: Field-scale economic-environmental trade-offs for a 90% compliance probability on a SCL (sandy clay loam) and SC (sandy clay) soil with a single and split fertiliser application.

Farm-scale economic-environmental trade-off case

The optimised baseline characteristics for farm-scale maize production are presented in **Table 5.4.** The total MAS for the unconstrained average N pollution output levels is R615 111. The baseline N pollution output levels become the start environmental targets in the compliance model runs.

Table 5.4: Optimised baseline for farm-scale maize production under 90 ha pivot consisting of 60 ha SCL (sandy clay loam) and 30 ha SC (sandy clay) soil.

		SCL	SC	Total
		Single	Single	
Margin above specified cost (MAS) (maximised)	R	401 074	205 037	615 111
Maize yield	ton	378	183	561
Nitrogen fertiliser used	kg	9 240	4 860	14 100
Irrigation water applied	-	501 mm	488 mm	44 700 m^3
N Pollution output level	kg/a	1518	777	2 295
Area planted	ha	60	30	90

Farm-scale economic-environmental trade-off curves presented in **Figure 5.12** illustrate the relationship between trade-off, environmental targets and compliance assurance/probability. As the compliance probability decreases, an increased frequency of exceedences of any specific pollution target is allowed. The decrease in MAS is much less at lower compliance probabilities; for instance, for Target_0, as compliance is relaxed from 90% to 40%, the MAS increases from R262 974 to R458 659. As the baseline pollution level is improved (moved towards Target_50), the difference in MAS due to lower compliance probability decreases, but the absolute reduction in MAS increases.

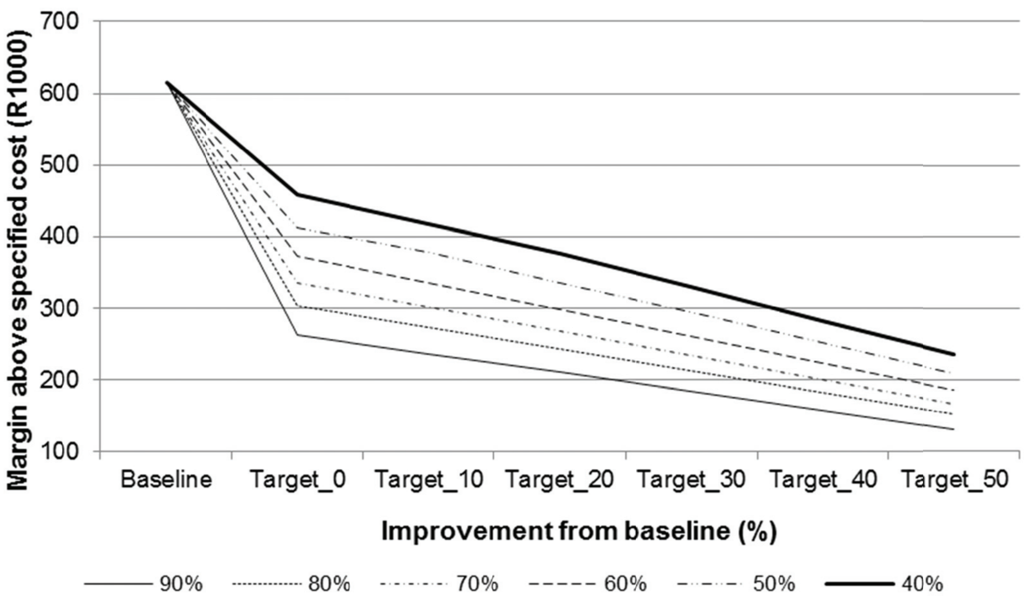

Figure 5.12: Economic-environmental trade-offs determined with the UPM at farm-scale for different compliance probabilities.

In general, faced with any increased constraint on the environmental outcome, i.e. more stringent environmental target or more stringent compliance probability or both, the farmer needs to change his/her production practices and/or pollution controls to maintain the environmental outcome. Such measures usually increase costs or decrease income, hence the decrease in MAS.

Catchment-scale economic-environmental trade-off case
The optimised baseline characteristics for catchment-scale sugar cane production in the Mkabela catchment are presented in **Table 5.5**. The total MAS for unconstrained pollution output (no control/mitigation measures) is R33.573 million. The baseline pollution output levels become the start environmental targets in the compliance model runs.

Table 5.5: Optimised margin above specified cost (MAS), area planted and pollution levels for the baseline catchment-scale model

Land Segment	Margin above specified cost (R million)	Area planted (ha)	Margin above specified cost (R/ha)	Baseline pollution output level (kg/ha/a)		
				Nitrogen	Sediment	Phosphorus
LS1	6.884	631	10 910.	2.15	8.63	15.55
LS2	6.120	567	10 794.	8.16	6.76	2.28
LS3	7.919	732	10 819	10.75	7.60	12.08
LS4	12.648	1 169	10 819	10.48	38.48	23.56
Total	33.573	3 099				

The following four pollution control scenarios were evaluated with the catchment compliance model:

- Scenario B_C: riparian buffers and field contours.
- Scenario B_NC: buffers but no field contours
- Scenario NB_C: field contours but no buffers.
- Scenario NB_NC: no buffers and no field contours.

The compliance model was used to model 100% compliance ("safety first rule") with each selected environmental target for the four pollution control scenarios. The compliance model was run separately for every pollutant in the catchment. For the sake of economy the results of only the N pollution case is discussed in detail here. The findings for sediments and phosphorus largely mimic those for N.

Figure 5.13 shows that the economic-environmental trade-offs for improving N pollution at catchment-scale are almost linear. Scenario NB_NC is a situation where no buffer/contour control measures are used to mitigate N pollution. The only way to reduce nitrogen pollution in such a case would be to reduce nitrogen applications per hectare or to plant less sugarcane. As a result, a significant reduction in MAS of R3.75 million was modelled for the case where baseline N pollution levels were reduced by 50%. When introducing buffers (B_NC), the trade-off between compliance and MAS improved a little – by R0.29 million at the Target_50 level.

The use of contours during the simulation of sugar cane production in *ACRU-NPS* reduced N pollution to levels below the environmental targets specified, even below the stringent Target_50; therefore, no trade-offs were necessary for compliance and, thus, the estimated MAS for scenarios B_C and NB_C remained constant at the baseline value.

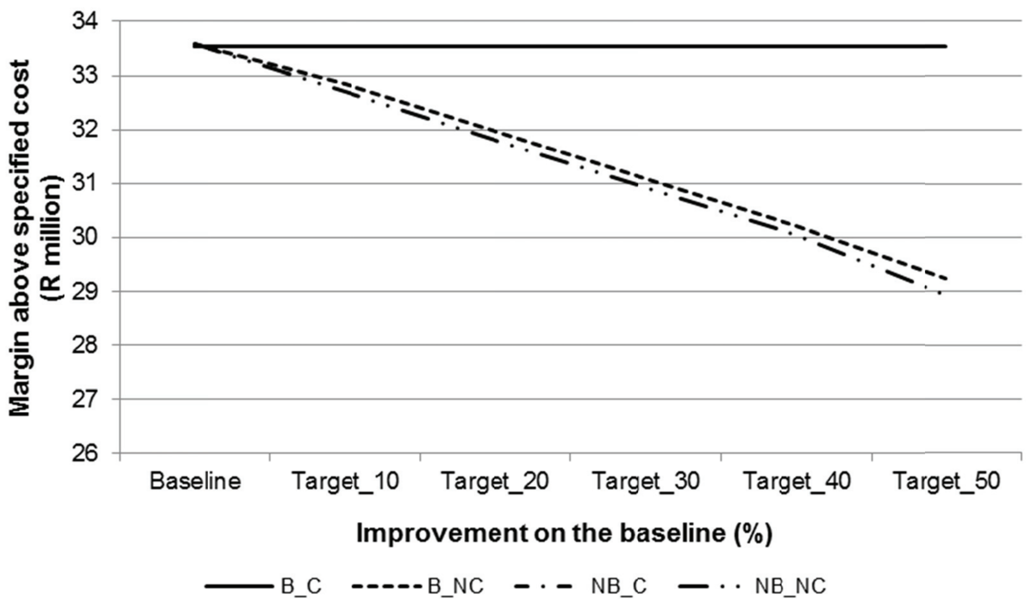

Figure 5.13: Economic-environmental trade-offs for increased abatement of N pollution from the Mkabela catchment for scenarios B_C, B_NC, NB_C, and NB_NC.

Comparing scenarios B_C to B_NC and NB_C to NB_NC the conclusion is that contours contribute substantially to the abatement of N pollution from sugarcane fields and to a "defence" of the MAS in a situation of environmental compliance. Furthermore, the value of such contours is illustrated by the difference between scenario B_C and B_NC, or, when no buffers are used, scenarios NB_C and NB_NC. On average the benefit amounts to R3.6 million. Although the use of buffers does mitigate nitrogen pollution, buffers are not as valuable in trade-off terms to reduce nitrogen pollution as contours are.

6 LESSONS LEARNT

6.1 Overarching Project Learnings

i. This Project demonstrated that combining researchers in Economics with bio-physical scientists in Agriculture and Hydrology in long-term, multi-scale, multi-disciplinary research, is not only operationally feasible, but also yields notable scientific and technological returns. These returns are shaped by the resulting cross-discipline reality-checks on each other's priorities and target outcomes, the resulting "conceptual stretch" imposed on prior discipline-rooted thought and attitude, and various "organic" manifestations of knowledge-seeding across discipline boundaries.

ii. The trajectory of this multi-scale, multi-disciplinary research was shaped by the original intention for this Project, as expressed by the opening phrase in its formal title: "*development of an integrated modelling approach to prediction.....*". In the course of their seven-year-long engagement with the Project, during periods of intense challenge or frustration, the senior members of the Project Team repeatedly revisited this phrase for succour and refocusing. We had to remind ourselves that the focus should be on developing an "approach" and not the ultimate "predictive tool-box". We learned, incrementally, that the term, "approach", required from us a dynamic process, not a static product, and a "learning-by-doing", rather than a pre-determined sequence of closely-specified tasks.

iii. There can never be too much face-to-face scientific engagement and work-sharing across the participating Teams if the "stretch" demands imposed by the term, "integrated" (in the above opening phrase), were to be satisfied. This Project included four annual Task Team Workshops, three joint field visits, six Reference Group meetings and more than a dozen mini-workshops and brainstorming sessions in which sub-groupings of the respective Research Teams participated. Yet, we have to recognise that in reality integration occurred only intermittently and that continuous integration remained a somewhat elusive achievement for this Project.

iv. The most striking integration moments occurred during the various stages of interfacing of the economic-environmental trade-off modelling with the bio-physical modelling, during the last 18 months of the Project. In these particular moments the bio-physical and economics researchers had to "get into each other's heads", as was remarked by one of the participants. Another remarkable integrating moment was when the whole Project Team intensively discussed the best way forward for the pesticide modelling research, after a disheartening finding concluded the early inception research on existing pesticide models. That finding was that this Project would not have the resources to do justice to the developments required to take pesticide modelling to a new level. This discussion resulted in a joint decision that the Pesticide Team would rather focus on an expert system that would be an improvement over existing expert systems – which, in turn, led to the highly successful development of PestEx.

v. It was highly advantageous that the Project leadership and administrative coordination functioned independently of the four Specialist Task Teams. This ensured that both strategic and pragmatic decisions about and responses to project developments and financial allocations could be relatively free of conflict of interest complications.

vi. Although organised agriculture was represented on the Reference Group for this Project, a broad engagement with farmers and related stakeholders was not attempted, given the highly scientific-technical nature of the Project and its stringent budget limitations. Any research follow-up to this Project should incorporate such broad "external" engagement.

6.2 Team: Economics of Agricultural NPS Pollution Management

6.2.1 Research Design

i. Trade-off models can provide powerful support to multi-disciplinary research projects to quantify and assess competing objectives in agricultural production or environmental management systems. A trade-off curve is a concrete visualisation of the instinctive mental optimisation calculations of experienced public decision-makers (Stoorvogel, Antle, Crissman and Bowen, 2001). During multi-disciplinary research projects complex bio-physical and economic models need to be developed to evaluate such trade-offs. The economic models are reliant on outputs of the bio-physical simulation models. Thus, in this Project, the research design of the Economics Task was to a large extent determined by the capabilities of the bio-physical simulation models to simulate the effects of management options and structural interventions to control NPS pollution loads.

ii. Johansson, Gowda, Mulla and Dalzell (2004) illustrated the use of a meta-model for integrating complex bio-physical and economic analyses to allow greater flexibility in policy analysis, both from the cost-side and from the abatement-side. According to Johansson et al. (2004), several authors have promoted 'meta-modelling' as a means to synthesise these detailed bio-physical and economic analyses in a policy-relevant framework. Primary lessons learnt by the Economics Team were the need to develop economic meta-models that reflected the cause/effect relationships of the processes that govern NPS pollution and how to synthesise the outputs from the aforementioned simulation models to populate the meta-models.

6.2.2 Multi-Team/Multi-Location Integration and Collaboration

iii. The Economics Team was dependent on extensive modelling support and technical interaction with the Nutrients/Field-Scale Team and Catchment-Scale Team. Typically, the developers of bio-physical simulation models in the agricultural domain primarily focus on simulating nutrient uptake and losses from the soil or within the system being modelled. Less attention is generally given to simulating crop production, which results in strong empiricism in crop yield estimation and not the same degree of mechanistic process formulation on the crop production side of bio-physical models. From an economics perspective, validating simulated crop yield is essential, since the interaction between management practices and their effect on crop yield provides the necessary link to the economics. Model developers might get overwhelmed by the physical and chemical processes that govern NPS pollution, so that the interaction with crop yield is neglected. Therefore, frequent and in-depth interactions between the economics and bio-physical modelling teams is essential for reliable modelling of economic-environmental trade-offs. Such interactions need to start early on the bio-physical model development trajectory to ensure alignment of technical priorities.

6.2.3 Interfacing Natural Resource Management Needs and Scientific Realities

iv. The economic-environmental trade-off models developed during this Project can be used to transfer knowledge regarding appropriate environmental management practices to Agriculture stakeholders and Environmental Management practitioners. Additionally, the trade-off modelling outcomes can also serve to sensitise and inform such stakeholders and practitioners as to the bigger picture of balancing sustainability and production.

v. It is important to note that economic-environmental trade-offs can only be quantified for management alternatives that can be satisfactorily simulated with the bio-physical models. Furthermore, the procedure used to represent the layout of the catchment in the economic model is not generic and, therefore, the catchment-scale economic model is not transferable to other case study areas. Reliable and stable mathematical programming and softwarecoding expertise is thus required to reconfigure the economic models for each case and to generate the relevant trade-offs.

6.3 Team: Nutrients and Field-Scale Modelling

6.3.1 Research Design

i. The FAIM-based research design (see Section 3.1) ensured a timely focus during the Nutrients Task on acquisition of reliable data sets for testing of applicable existing or new algorithms and models and, especially, the establishment of a lysimeter-based crop production trial customised to the objectives of this Project. This focus underlined an ongoing need to maintain an up-to-date "library" of reliable international laboratory and field experiments in the nutrient dynamics and crop production domains.

ii. The lack of reliable, adequately detailed parameterization data has been a common limitation to bio-physical model application internationally (Sharpley, 2007). During the SWB-Sci model development phase under this Task, it became clear that, obtaining P initialization soil parameters for South African soils, was highly challenging. Therefore, specific guidelines were developed in this Project to assist model users in the parameterization of South African soils. The guidelines, published as a scientific paper (Van der Laan et al., 2009), enable modellers to utilize land type maps, which are available for the whole of South Africa at a scale of 1:250 000 (including the accompanying Memoirs), to parameterize both field- and catchment-scale models. These guidelines could only be brought about by a truly trans-disciplinary and multi-scale effort, which the Project's research design promoted and facilitated.

iii. During the initial testing of the SWB-Sci model, after its initial augmentation with "borrowed" algorithms for nutrient dynamics, the Nutrients Team soon realised that an improved approach to simulate the effect of N stress on crop yield was essential. Therefore, a new approach was conceptualised and implemented in which the effect of N stress on crop yield was simulated on a daily basis following flowering, as opposed to simulating the effect of N stress on a "harvest index" as used in the earlier "borrowed" algorithms for nutrient dynamics. During tests of the improved model against observed nutrient dynamics datasets from the Netherlands and South Africa, the new SWB-Sci model was judged to simulate N dynamics in cropping systems more than adequately.

6.3.2 Approaches to Scaling

iv. The modelling of NPS N and P pollution is undertaken at different spatial scales. Numerous views are expressed in the related literature on the dimensions of different scales, but point- (~1 m^2), plot- (~25 m^2), hillslope- (~1 ha), field- (broadly defined), small catchment (~1 km^2), and large catchment (~1000 km^2) scales are often referred to (Quin, 2004). In this Project field-scale is viewed as a scale with dimensions of about 1 ha, which is still suitable for simulation by a one-dimensional bio-physical model.

v. The following principles guided model upscaling from field- to catchment-scale in this Project in order to capture important N and P processes in the simulation:
   - certain processes reflect a dominant response for nutrient dynamics at different scales
   - the modelling of larger areas necessitate the aggregation of selected input parameters
   - the larger scale enforces a more empirical content to algorithms
   - sufficient complexity must be captured to properly account for the mass balance at catchment-scale.

vi. In efforts towards upscaling, two different general approaches are possible. The first comprises the close-coupling of detailed field-scale model simulation output to catchment scale models (Andresson et al. 2005). The second is integrating simplified process parameterisations into the catchment-scale model. It is important not only to include processes for which parameters can be determined at catchment-scale, but also to avoid simplification which will inhibit the ability to conclude source-pathway-response modelling. For catchment-scale modelling in this project, the second approach was adopted, in which nutrient process responses from the GLEAMS model were incorporated into the *ACRU-NPS* model and then refined where necessary.

vii. A crucial component of both upscaling and downscaling in the Project was the development of customised scientifically-based guidelines needed by model users in the parameterization of South African soils and published as a scientific paper – Van der Laan et al. (2009) – already outlined in Section 6.2.1.

viii. Due to the mechanistic nature of SWB-Sci, and because much work has been done on a variety of crops in South Africa with the model, the SWB-Sci can be used to generate crop input parameters such as potential yield and LAI under non-limiting conditions for the catchment-scale model. Additional parameters that can potentially be obtained through the running of simulations with SWB-Sci include the amount of crop residue remaining on the land after harvest and the decline in soil organic matter over time due to cultivation. A comparison of SWB-Sci and *ACRU-NPS* or SWAT – in which simulations are run for a single scenario at an intermediate scale – can provide insight into the ability of each model to simulate various processes and highlight strengths/weaknesses of each model. Ultimately, it is envisaged that SWB-Sci should play an important role in cross-checking of processes in the catchment-scale models.

6.3.3 Interfacing Natural Resource Management Needs and Scientific Realities

ix. Technological advances and an increase in computer availability have resulted in widespread development of mathematical models that simulate nutrient dynamics in cropping systems. Despite this, "examples of real impacts of these modelling efforts on current farming practices are rare" (Carberry et al., 2002). Mechanistic crop models have played a role in greatly enhancing our understanding of nutrient dynamics, and according to McCown et al. (1992), such models can assess fertiliser use in a way not feasible using long-term trials on their own. Carberry et al. (2002) discussed four case studies where bio-physical models were used to improve understanding in nutrient use efficiency and found evidence that models could be utilized to contribute to significant changes in management practices for commercial farmers. In applying the Agricultural Production Systems Simulator (APSIM) model to maize/legume systems in Africa, Whitebread et al. (2009) identified four distinct modes of use: (1) to add value to experimentation, (2) to facilitate direct engagement with farmers, (3) to explore system constraints and opportunities with researchers and extension officers, and (4) to generate information for policy makers and financial institutions.

x. SWB-Sci is well positioned for significant contributions in any of the above four modes of use. As a minimum, it is envisaged that SWB-Sci should play an important role in determining best nutrient management practices at the field/farm management level; such as conducting simulations to analyse critical N and P leaching periods for different cropping systems. This would lead to the identification of critical nutrient export areas and effective management practices to reduce these losses. In addition, such modelling should also assist in the planning of field trials and monitoring programmes to further enhance our understanding of these matters.

xi. Capacity to model nutrient dynamics in cropping systems at the point- to field-scales has perennially been lacking in South Africa. Through this Project and the incorporation of N and P into SWB-Sci, three PhD students based at the University of Pretoria's Department of Plant Production and Soil Science have become actively involved in this type of modelling, resulting in a significant increase in scientific capacity with regards to both modelling software and skills development.

6.4 Team: Pesticide Modelling

6.4.1 Research Design

i. The required baseline data for catchment monitoring of NPS pollutants should include geology and hydrogeology, soils, climate, hydrological data (volumes and quality), as well as history of land use, fertilization, pesticide application and land management. It is imperative that monitoring should include all components of the system, namely atmospheric, soil, surface water and groundwater.

ii. Due to the large number of chemicals applied to protect crops, where each of these chemical species has specific properties (volatilization, sorption and degradation), it is recommended that a target spectrum of pesticides be detected at key locations in catchments in order to identify priority species to be monitored.

6.4.2 Approaches to Scaling

iii. The team consisted of researchers and collaborators with complementary expertise in different fields and modellers at different spatial scales. Since the start of the project, modelling and remote sensing capabilities have improved to the point that integration of detailed information at field-scale into large catchment-scale has now become a realistic goal. Intensive monitoring at field-scale of water and nutrient fluxes can therefore serve the purpose of informing processes at catchment-scale. In order to achieve this, it is imperative that databases of detailed information be compiled in order to facilitate the set-up and parameterization of distributed hydrological models operating according to the principle of hydrological response units (e.g. ACRU). The database population and handling will be crucial.

6.4.3 Interfacing Natural Resource Management Needs and Scientific Realities

iv. The predictive capabilities of existing models/methods and those developed during the course of this project can be used to transfer knowledge to water managers and to work with water managers. In particular, scenarios of land use and management can be simulated to recommend the most environmentally and economically acceptable practices. It is, however, essential that these scenarios be developed through a participatory approach with stakeholders (scientists and modellers, farmers, Government officials and others) in order to facilitate knowledge transfer.

6.5 Team: Catchment-Scale Modelling

6.5.1 Research Design

i. Research design could have included more case studies with associated observations of water, sediment, nutrient and pesticide dynamics. Significant time and energy went into questioning only two research sites and a small number of land uses rather than a cross section of many land uses and crop types. Clearly, the second option would have suited the field-scale team, but multiple research sites were infeasible for catchment-scale observations.

6.5.2 Multi-Team/Multi-Location Integration and Collaboration

ii. The team benefited from interaction between field-scale nutrient research and the catchment-scale model development. More frequent scientific interaction earlier in the project would have been beneficial. The lack of appropriately detailed measurements in the

Mkabela research catchment for small-scale verifications limited the interaction between field- and catchment-scale process algorithm development.

iii. Research of non-point source pollution from field- to catchment-scales requires multidisciplinary integration and continuous collaboration. Research efforts stagnate without frequent communication and comparison/distribution of input data and simulated outputs. Another challenge in this regard relates to the timescale of the Project (over 5 years). Long-term projects require research to be conducted intermittently, making it a challenge to keep focussed and up to date with other teams. An additional challenge is the timeous comparisons of one's own research findings with those of other teams, especially when they operate at different locations and scales.

6.5.3 Approaches to Scaling

iv. Dividing the Project Team into smaller Teams to focus on specific scales was important. The nested catchment was an ideal site for interaction of the Teams and to study mass transport dynamics from point- to field- to catchment-scales. However, insufficient detail in measurement at the field-scale, particularly soil profile nutrient dynamics, as well as infrequent observation of discharge at the larger scale, limited some aspects of model testing. Because the Project budget was insufficient for these additional observations, they were done on an ad hoc basis. Nevertheless, significant contributions to the understanding of the fate of nutrients and sediments from source to catchment-scale were made from observations in the catchment and from applying the models to this catchment.

v. Models such as SWAT and *ACRU-NPS* can be defined as distributed lumped-parameter models that aggregate representative processes over the scale at which outputs are simulated However, aggregating land-use/soil combinations disregard small but important sediment- or nutrient-producing areas (e.g. a small vegetable plot). This should be catered for through sub-catchment delineation into hydrological response units (HRUs) to capture the diversity of land use within sub-catchments. HRUs are portions of a sub-catchment that possess unique land use/soil attributes (Neitsch et al., 2000). Inclusion of multiple HRUs allow simulations to account for this diversity and to identify small but important source areas of erosion, e.g. a cabbage farm with relatively poor crop cover with higher (20 to 50 times) sediment and nutrient rates than areas with good canopy and ground cover (forestry).

6.5.4 Interfacing Natural Resource Management Needs and Scientific Realities

vi. The development of bio-physical models in this Project which do not only predict sediment and nutrient delivery at different scales of interest, but also associated crop yields, ought to be invaluable to agricultural production and environmental management stakeholders. Inclusion of sufficient scientific complexity into the models to allow for realistic predictions of NPS pollution loads as well as crop yields has been a primary intention of this Project. However, such a claim will have to be tested against different cropping and agricultural pollution control/mitigation systems.

vii. Given their complex nature and input requirements, the models developed by the scientists in this Project cannot be handed over for general use by natural resource managers, but the Team has demonstrated how useful scenarios can be developed to inform agricultural production and environmental management decision-making.

7 FUTURE RESEARCH PRIORITIES IN AGRICULTURAL NPS MODELLING AND ECONOMICS OF AGRICULTURAL NPS MANAGEMENT

7.1 Team: Economics of Agricultural NPS Pollution Management

i. Due to the interaction between crop yield, applied irrigation water and pollution loads it might be beneficial to estimate the nitrogen response functions used in the economic models simultaneously. One way is to use "seemingly unrelated regression equations" – SURE. Although the models could be estimated equation-by-equation, it could be more appropriate to use SURE to find more consistent estimates. However the use of a SURE approach is based on the assumption that the error terms for the equations are correlated. Alternatively, the use of causality models can be investigated. It can be argued that an increased level of pollutant emissions can be caused by poor crop growth and increased water use. Although no relationship between irrigation water applied and nitrate emissions was evident in this study, this cannot always be assumed to be the case.

ii. The Upper Partial Moment (UPM) method used to determine the economic-environmental trade-offs at field- and farm-scale is highly conservative. The conservativeness of the model results from the fact that the procedure satisfies the environmental constraint at a higher than specified probability level. Future research should address the conservatism of the UPM.

iii. Apart from the conservativeness of the UPM method, more interaction with policy-makers or environmental regulators is required to establish the level at which environmental standards need to be maintained. The linked bio-physical/economic modelling framework paves the way for the evaluation of alternative policy instruments to achieve environmental goals. Research is also necessary to determine the interaction between maintaining a single environmental goal against simultaneously maintaining environmental goals for different pollutants.

iv. The economic catchment-scale programming model should be further developed into a generic model, which would aid the transferability of the model to other case studies and locations.

v. Pollution risk was not considered in this study due to data limitations. The model should be further developed to incorporate the distribution of NPS pollution loads. The procedures developed by Richardson et al. (2000) should be explored as a means to derive stochastic contribution coefficients.

7.2 Team: Nutrients and Field-Scale Modelling

i. The approach proposed to categorize South African soils as 'slightly weathered', 'highly weathered' or 'calcareous' at the catchment scale is open to further discussion and debate. While it is acknowledged that topsoil characteristics such as sum of bases, presence of $CaCO_3$ and acidity can easily be modified through fertiliser or lime applications to cultivated land, in South Africa only 10% of land is under cultivation. In most cases, modal profiles were in native land and soil characteristics would not have been expected to be modified by past agricultural practices. An uncertainty using this approach is whether small cultivated areas with high soil P in a catchment contribute comparable pollutant loads to larger areas with lower soil P. Therefore although by no means a faultless suggestion, it is meant to be a pragmatic approach considering the lack of detailed soil information at catchment scale, and the urgent need to estimate the impacts of land use and management strategies on eutrophication of inland waterways and impoundments. Further research on P dynamics in South African soils is therefore essential in testing the guidelines suggested for soil parameterization as provided in this study.

ii. Crop N and P models often use approaches that can differ vastly in complexity to simulate N and P dynamics in cropping systems. This leads to various strengths and weaknesses for a particular model. For a model to be considered mechanistic, the cropping system being described at one level must be described by processes operating at a lower level (Sinclair and Seligman, 2000). In reviewing 14 N simulation models, De Willigen (1991) observed that above-ground variables (yield, grain N mass) were better simulated than below-ground variables (soil water and mineral N content) and concluded that simulating soil biological processes is the most problematic. This most likely also applies for P. It is therefore suggested that work done to improve the capability of point/field scale models to accurately simulate N and P dynamics in cropping systems be focused on below-ground processes, most notably inorganic N processes, organic matter cycling processes, soil matrix – P interactions, and solute leaching (discussed further below). Such work would, for example, include accounting for the influence of a stony fraction in the soil on the above-mentioned processes in SWB-Sci.

iii. Despite an improved understanding of P sources and transfer pathways since early work done by Jones et al. (1984) and Sharpley et al. (1984), models are often not updated adequately to reflect these new insights (Sharpley et al., 2002; Vadas et al., 2006). Radcliffe and Carberra (2007) suggested that with recent research showing that leaching can be an important subsurface pathway for P losses, improved description of P leaching in models is required. Related to this, the vertical leaching of organic N and P attached to colloidal particles is currently not simulated in SWB-Sci, *ACRU-NPS* or SWAT. A significant movement of N and P via vertical leaching and/or lateral flow may potentially be missed by excluding this process, especially under systems receiving high loadings of organic material. Similarly, the simulation of N and P leaching via macropore flow should be considered in future model versions.

iv. Results from this study demonstrate that pollution mitigation/control measures can significantly reduce N leaching from irrigated agriculture, but not to levels observed for dryland production. Further research considering unit leached per unit yield will assist in further improving comparisons of dryland and irrigated agriculture with regards to nutrient pollution potential.

v. Continued research and monitoring work is needed to collect nutrient export data from agricultural systems. This will lead to improved model calibration and refinement of the algorithms used in the various models.

vi. Freshly mineralized inorganic N is clearly an important contribution to crop available N, and development of a simple laboratory procedure to obtain these values could be highly beneficial to SBW-Sci model users.

vii. Using a dryland maize dataset collected in Kenya, SWB-Sci simulated aboveground dry matter production (TDM), yield, leaf area index (LAI), profile water content, aboveground N and P mass, and grain N and P mass with varying levels of accuracy. Unfortunately, soil N and P levels had not been measured in this trial, which made testing and comparison of measured and simulated values more difficult. Except for aboveground P mass, agreement between measured and simulated values was almost always better for the first growth season than for the second growth season. Exact reasons for poorer performance by the model during the second season are not immediately clear. There could have been something that happened in the field when transitioning from the one season to the next that is not adequately captured in the simulations, or some of the newly developed algorithms still need further improvement; therefore, further testing and refinement of these newly included algorithms is recommended.

7.3 Team: Pesticide Modelling

i. A lack of sound data sets for modelling pesticides at different scales was an expected shortcoming. Pesticides are chemicals with highly focused properties and new products are continuously being released on the market. It is essential that a national monitoring programme of pesticide fluxes in critical catchment locations, as well as ecotoxicological studies be continuously strengthened and rationalized.

ii. PestEX should be physically-chemically calibrated and validated in a range of soil/environment combinations, crop cultivations and for different pesticides.

iii. Soil quality is an emerging discipline that aims at integrating the traditional disciplines in soil sciences, namely soil physics, soil chemistry, soil biology and pedology. Soil quality assessment was beyond the scope of this project. However, an anecdotal occurrence points to a research need, as follows: During the data collection campaigns in the Goedertrou experimental catchment in 2005, soil samples were collected for laboratory analyses of pesticides. The laboratory at the Plant Protection Research Institute at Roodeplaat (Agricultural Research Council) could not determine pesticides in those samples due to the presence of other organic compounds, possibly hydrocarbons, masking the pesticide signals in the spectral analysis. The suspected source of hydrocarbons could be agricultural machinery previously used in the catchment. This occurrence triggers the question: What are all the unknown factors (e.g. residual pesticides, hydrocarbons, etc.) that could affect food production and ultimately impact on sustainable use of soil and water resources? In that sense, it would be highly beneficial to initiate a broad soil quality research programme in order to define and quantify soil quality indicators and thresholds for different environmental conditions, as well as to describe and quantify interactions of physical, pedogenetical, chemical and biological soil processes, as these are likely to affect water resources directly or indirectly.

iv. Integrated pest management or alternative methods of pest control are also in the initial stages of research and do require much more attention in future.

7.4 Team: Catchment-Scale Modelling

Observations and Process Understanding

i. Observations are required at a smaller time resolution at the larger scale in order to estimate event nutrient and sediment loads in the nested catchment and thus an accurate evaluation of the losses or gains through the network;

ii. In-situ and laboratory observations and quantification of the subsurface migration of phosphorus and assessment of surface and subsurface phosphorus species pathways from field to stream;

iii. Observations and quantification of subsurface controls of water and nutrient pathways in land forms;

iv. Observation and quantification of nutrient and sediment detention, retention or reaction in specific controls in stream networks, including farm dams, wetlands and buffer strips subject to a range of rainfall/runoff events;

v. Verification of nutrient uptake processes under various stressed and unstressed conditions;

vi. Observation and quantification of water and nutrient movement in the vadose zone, recharge to groundwater and subsequent migration. The use of hydropedological surveys could be used to enhance the definition of nutrient pathways.

Model Development and Comparison

vii. Continued development of the use of land type and hydropedological surveys to estimate model parameters for water, sediment and nutrient simulation;

viii. Development of response functions to simulate the time distribution of water and nutrient migration in surface and subsurface flows. These response functions should be developed from in-situ observations as well as simplified from local or field scale algorithms;
ix. Verification of simulated nutrient uptake and crop yield responses to water and nutrient stress and recovery through observation;
x. Include in the modelling, secondary effects of scenario options, such as: effect on vegetation cover and yield in scenarios in which erosion is enhanced; effect on the yield of the removal or inclusion of in-field remedial measures and visa versa, the effect on sediment yield and nutrient loads resulting from stressed crop growth.
xi. Use and evaluation of the model systems in ungauged basins;
xii. Comparison of specific model features, such as the wetland, buffer and small dam routines; the Green-Ampt infiltration versus the SCS runoff generation options (both inherent in ACRU-NPS and SWAT) and subsurface processes simulations;
xiii. Evaluation of sensitivity of simulated sediment and nutrient loading to disaggregation versus lumping of land segments.

8 THE WAY FORWARD

This Project demonstrated that combining economic and applied natural sciences in long-term, multi-scale, multi-disciplinary research is not only operationally feasible, but also yields notable scientific and technological returns. Apart from numerous cross-disciplinary research process learnings and the somewhat subtle knowledge-seedings mentioned in Section 6.1, various multi-scale and multi-disciplinary management decision-support and planning analysis modelling tools were established – albeit in provisional shapes in a number of respects. Inevitably, at the conclusion of this relatively long-duration, often taxing, sometimes frustrating, mostly fascinating, but, generally successful, research process, a vital question arose among the senior members of the Project Team, as follows:

> *Quo Vadis, South African research into the modelling of agricultural NPS pollution, coupled with the modelling of economic-environmental trade-offs?*

The Project Team, naturally, did not have a mandate to address such a future-seeking question in any significant manner; but, we did recognise that an appropriate response to such a vital question would need to be based on cognisance of the "lessons learnt" and the "future research recommendations" stemming from this project (presented in Sections 6 and 7, respectively), as well as of the findings of numerous current or recent related, overlapping, or supporting research initiatives in the RSA and internationally.

Given the above context, the following "Way Forward" is proposed:

- A Scene-Setting/Research-Planning Workshop to derive research priorities from examination of the local and international state-of-the-art of research regarding NPS pollution and its modelling, with a specific focus on Agriculture, its relationship with Environmental Management and the related Economics of Environmental Compliance.
- A follow-up Research Project regarding Agricultural NPS Pollution Management of a long-term, multi-scale, trans-disciplinary nature that would encapsulate in a systematic, integrated manner, the 34 "lessons learnt" reported in Section 6 and the 29 "future research recommendations" formulated in Section 7, as well as fresh priorities indicated by advances in recent or overlapping related local and international research, as gleaned from the above Scene-Setting/Research-Planning Workshop.
- This follow up Project would need to comprise a range of trans-disciplinary approaches that would facilitate ongoing broad engagement by the research team with farmers, agricultural extension officers, officials in regulatory roles, agricultural and environmental planning officials, related policy-makers and related NGOs. An objective should be that pollution management practices, solutions, planning and policy-implementation should be influenced to change while the science is still being done!
- The funding requirements of such a long-term trans-disciplinary Project would be significant and would probably need to come from a range of sources including the WRC, the government departments dealing with water, environment and agriculture, and international development aid agencies.

The arrow-of-time has in recent years imparted a unique momentum to the South African pursuit of advances in NPS pollution management. The new research undertakings proposed above would markedly increase the existing momentum and be able to build effectively on the promising outcomes created by the Project described in this Overview Report.

9 REFERENCES

General

PEGRAM GC and GöRGENS AHM (2001) *A Guide to Non-Point Source Assessment in South Africa*. WRC Report No. TT 142/01. Pretoria, South Africa.

ROSSOUW JN, CULLIS J and GöRGENS AHM (2005) *Knowledge Review of Modelling Non-Point Source Pollution in Agriculture from Field to Catchment Scale*. WRC Report No. 1467/1/05. Pretoria, South Africa.

CULLIS J (2005) *First Order Estimate of the Contribution of Agriculture to Non-Point Source Pollution in South Africa.* WRC Report No. 1467/2/05. Pretoria, South Africa.

Team: Nutrients and Field-Scale Modelling

ANDERSSON L, ROSBERG J, PERS BC, OLSSON J and ARHEIMER B (2005) Estimating catchment nutrient flow with the HBV-NP model: Sensitivity to input data. *Ambio* **34** 521-532.

ANNANDALE JG, BENADE N, JOVANOVIC NZ, STEYN JM and DU SAUTOY N (1999a) *Facilitating irrigation scheduling by means of the Soil Water Balance model.* WRC Report No. 753/1/99. Pretoria, South Africa.

ANNANDALE JG, CAMPBELL GS, OLIVIER FC and JOVANOVIC NZ (1999b) Predicating crop water uptake under full and deficit irrigation: An example using pea (*Pisum sativum* L. cv. Puget). *Irrig. Sci.* **19** 65-72.

ANNANDALE JG, JOVANOVIC NZ, TANNER PD, BENADE N and DU PLESSIS HM (2002) The sustainability of irrigation with gypsiferous mine water and implications for the mining industry in South Africa. *Mine Water Env.* **21** 81-90.

CAMPBELL KL, KIKER GA and CLARK DJ (2001) Development and testing of a nitrogen and phosphorus process model for Southern African water quality issues. ASAE Annual International meeting. *Paper No. 012085*, St. Joseph, MI.: ASAE.

CARBERRY PS, PROBERT ME, DIMES JP, KEATING BA and MCCOWN RL (2002) Role of modelling nutrient efficiency in cropping systems. *Plant Soil* **245** 193-203.

CORWIN DL, WAGGONER BL and RHOADES JD (1991) A function model of solute transport that accounts for bypass flow. *J. Environ. Qual.* **20** 647-658.

DAROUB SH, GERAKIS A, RITHCIE JT, FRIESEN DK and RYAN J (2003) Development of a soil-plant phosphorus simulation model for calcareous and weathered tropical soils. *Agric. Sys.* **76** 1157-1181.

DE WILLGEN P (1991) Nitrogen turnover in the soil-crop system; comparison of fourteen simulation models. *Fert. Res.* **27** 141-150.

GITAU MW and VEITH TL (2007) Quantifying the effects of phosphorus control best management practices. In: Radcliffe DE and Cabrera ML (eds.) Modeling phosphorus in the environment. CRC Press, New York, USA.

GROOT JJR and VERBENE ELJ (1991) Response of wheat to nitrogen fertilization, a data set to validate simulation models for nitrogen dynamics in crop and soil. *Fert. Res.* **27** 349-383.

JONES CA, COLE CV, SHARPLEY AN and WILLIAMS JR (1984) A simplified soil and plant phosphorus model: I. Documentation. *Soil Sci. Soc. Am. J.* **48** 800-805.

JOVANOVIC NZ and ANNANDALE JG (2000) Crop growth model parameters of 19 summer vegetable cultivars for use in mechanistic irrigation scheduling models. *Water SA* **26** 67-76.

JOVANOVIC NZ, ANNANDALE JG and BENNIE ATP (2002) Calibration and validation of the SWB irrigation scheduling model for soybean [Glycine max. (L.) Merr., indeterminate cv. Wayne]. *S. Afr. J. Plant Soil.* **19** 165-172.

JOVANOVIC NZ, ANNANDALE JG and MHLAULI NC (1999) Field water balance and SWB parameter determination of six winter vegetable species. *Water SA* **25** 191-196.

KEATING BA, CARBERRY PS, HAMMER GL, PROBERT ME, ROBERTSON MJ, HOLZWORTH D, HUTH NI, HARGREAVES JNG, MEINKE H, HOCHMAN Z, MCLEAN G, VERBURG K, SNOW V, DIMES JP, SILBURN M, WANG E, BROWN S, BRISTOW KL, ASSENG S, CHAPMAN S, MCCOWN RL, FREEBAIRN DM and SMITH CJ 2003 An overview of APSIM, a model designed for farming systems simulation. *Eur. J. Agron.* **18** 267-288.

KNISEL WG (Ed.) (1980) CREAMS: A field-scale model for Chemicals, Runoff and Erosion from Agricultural Management Systems. *U.S. Department of Agriculture, Science and Education Administration, Conservation Research Report No. 26.*

MCCOWN RL, KEATING BA, PROBERT ME and JONES RK (1992) Strategies for sustainable crop production in semi-arid Africa. *Outlook Agric.* **21** 21-31.

MULLER S and GREGORY J (2003) Ground Water Loading Effects of Agricultural Management Systems. University of Florida, Department of Agricultural and Biological Engineering.

NEITSCH SL, ARNOLD JG, KINIRY JR, WILLIAMS JR and KING, KW (2002) Soil Water Assessment Tool Theoretical Documentation. Grassland, Soil and Water Research Laboratory, Temple, Texas. *GSWRL Report 02-01*.

PROBERT ME and OKALEBO JR (1992) Effects of phosphorus on growth and development of maize. In: Probert ME (ed.) A Search for strategies for sustainable dryland cropping in semi-arid Eastern Kenya: proceedings of a symposium held in Nairobi, Kenya, 10-11 Dec. 1990.

RADCLIFFE DE and CABRERA ML (2007) Suggestions to improve modeling of phosphorus. In: Radcliffe DE and Cabrera ML (eds.) *Modeling phosphorus in the environment.* CRC Press, New York, USA. 405-415 pp.

ROBBINS CH (1991) Solute transport and reactions in salt-affected soils. In: Modeling Plant and Soil Systems. *Agronomy Monograph* No. 31, ASA-CSSA-SSSA, 677 S. Segoe Rd., Madison, WI 53711, 365-395.

QUIN P (2004) Scale appropriate modelling: representing cause-and-effect relationships in nitrate pollution at the catchment scale for the purpose of catchment scale planning. *J. Hydrol.* **291** 197-217.

SCHMIDT CJJ (1993) Kwantifisering van die stikstofbalans op die Glen-Shorrocks gewassekotoop. Finale Projekverslag GB5111/32/8/10, Instituut vir Grond, Klimaat en Water, Pretoria.

SHARPLEY AN (2007) Modeling phosphorus movement from agriculture to surface waters. In: Radcliffe DE and Cabrera ML (eds.) *Modeling phosphorus in the environment.* CRC Press, New York, USA. 3-19 pp.

SHARPLEY AN, JONES CA, GRAY C and COLE CV (1984) A simplified soil and plant phosphorus model. II Prediction of labile, organic and sorbed phosphorus. *Soil Sci. Soc. Am. J.* **48** 805-809.

SHARPLEY AN, KLEINMAN PJA, MCDOWELL RW, GITAU M and BRYANT RB (2002) Modeling phosphorus transport in agricultural watersheds: Processes and Possibilities. *J. Soil Water Conserv.* **57** 425-439.

SMITH M, ALLEN RG and PEREIRA LS (1996) Revised FAO methodology for crop water requirements. *Proc. of the Int. Conf. on Evapotranspiration and Irrigation Scheduling*, San Antonio, Texas, USA. 133-140.

STÖCKLE CO, DONATELLI M and NELSON R (2003) CropSyst, a cropping systems simulation model. *Europ. J. Agron.* **18** 289-307.

TESFAMARIAM EH (2004) Modelling the soil water balance of canola *Brassica napus* L (Hyola 60). M.Sc. (Agric.) diss. Univ. of Pretoria, Pretoria, South Africa.

VADAS PA, KROGSTAD T and SHARPLEY AN (2006) Modeling phosphorus transfer between labile and nonlabile soil pools: Updating the EPIC model. *Soil Sci. Soc. Am. J.* **70** 736-743.

VAN DER LAAN M, ANNANDALE JG, DU PREEZ CC and LORENTZ SL (2009) Obtaining the parameters required to model labile P for South African soils. *S. Afr. J. Plant Soil* **26** 213-219.

VAN DER LAAN M, ANNANDALE JG, TESFAMARIAM EH, DU PREEZ CC, BENADÉ N, BRISTOW KL and STIRZACKER RJ (2012). *Modelling Nitrogen and Phosphorus Dynamics in Cropping Systems at the Field Scale*. WRC Report No. 1516/1/12, Water Research Commission, Pretoria.

WHITEBREAD AM, ROBERTSON MJ, CARBERRY PS and DIMES JP (2009) How farming systems simulation can aid the development of more sustainable smallholder farming systems in southern Africa. *Eur. J. Agron.* doi:10.1016/j.eja.2009.05.004.

WILLIAMS JR, RENARD KG and DYKE PT (1983) EPIC Erosion Productivity Impact Calculator: A new method for assessing erosion's effect on soil productivity. *J. Soil Water Conserv.* **38** 381-383.

Team: Pesticide Modelling

BOESTEN JJTI (1999) From laboratory to field: uses and limitations of pesticide behaviour models for the soil/plant system. *Weed Res.* **40** 123-138.

CROWE AS and MUTCH JP (1992) EXPRES: An expert system for assessing the fate of pesticides in the subsurface. *Environmental Monitoring and Assessment* **23** 19-43.

JOVANOVIC NZ, PETERSEN C, BUGAN RDH and VAN DER WALT E (2012). *Modelling the Fate of Pesticides: Primary Processes, Non-Point Source Data Collection and Guidelines*. WRC Report No. 1516/2/12, Water Research Commission, Pretoria.

KOVACH J, PETZOLDT C, DEGNI J and TETTE J (1994) A method to measure the environmental impact of pesticides. New York's Food Life Sci. Bull. 139. N.Y. State Agric. Exp. Stat., Geneva, N.Y., USA.

MEINHARDT HR (2003) *Evaluation of Predictive Models for Pesticide Behaviour in South African Soils*. Water Research Commission Report No. 999/1/03, Pretoria, South Africa.
NEUMANN M, BAUMEISTER J, LIESS M and SCHULZ R (2003) An expert system to estimate the pesticide contamination of small streams using benthic macroinvertebrates as bioindicators. Part 2. The knowledge base of LIMPACT. *Ecological Indicators* **2** 391-401.

REUS JAWA and LEENDERTSE PC (2000) The environmental yardstick for pesticides: A practical indicator used in the Netherlands. *Crop Protection* **19(8-10)** 637-641.

VAN DER WERF HMG and ZIMMER C (1998) An indicator of pesticide environmental impact based on a fuzzy expert system. *Chemosphere* **36(10)** 2225-2249.

DICKENS CWS and GRAHAM PM (2002) South African Scoring System (SASS) Version 5: Rapid bioassessment method for rivers. *African Journal of Aquatic Science* **27(1)** 1-10.

USHER B, PRETORIUS JA, DENNIS I, JOVANOVIC N, CLARKE S, CAVE L, TITUS R and XU Y (2004) *Identification and Prioritization of Groundwater Contaminants and Sources in South Africa's Urban Catchments.* Water Research Commission Report No. 1326/1/04, Pretoria, South Africa.

VAN GENUCHTEN MTH, LEIJ FJ and YATES SR (1991) The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils, Version 1.0. *EPA Report 600/2-91/065*, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.

ZADEH LA (1965) Fuzzy sets. *Inform. Control* **8** 338-353.

Team: Catchment-Scale Modelling

ARNOLD JG, SRINIVASAN R, MUTTIAH RS and WILLIAMS JR (1998) Large area hydrologic modeling and assessment. Part I: Model development. *Journal of the American Water Resources Association*, **34**: 7389.

BHAT KKS, FLOWERS TH, O'CALLAGHAN JR. Nitrogen losses and surface runoff from landspreading of manures. *Proc. Euro Eco Comm Program of research on effluents from livestock*, Wexford Ireland. May 20-22, pp 222-46. (1980)

CAMPBELL, K.L., KIKER, G.A. AND CLARK, D.J. 2001. Development and Testing of a Nitrogen and Phosphorus Process Model for Southern African Water Quality Issues. *American Society of Agricultural Engineers Annual International Meeting*, July/August 2001, Sacramento, California. Paper Number: 01-2085.

DE CLERCQ WP, FEY MV and JOVANOVIC NZ (2009) *Land Use Impacts on Salinity in the Berg River Catchment.* Report No. 1503/08, Water Research Commission, Pretoria, South Africa. In progress.

FAO (1998) *World Reference Base for Soil Resources*. Food and Agricultural Organization of the United Nations, Rome, Italy.

KNISEL, W.G. (ed.). *GLEAMS: groundwater loading effects of agricultural management systems, Version 2.10.* University of Georgia Coastal Plain Experiment Station, Publication No. 5 (1993).

KNISEL, W. G. AND F. M. DAVIS, 1999. *GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) Version 3.0 User Manual*. SEWRL-WGK/FMD-050199. Tifton, GA. 167 p.

LE ROUX, PAL, FRAENKEL, CH, BOTHMA, CB, GUTTER, JH AND DU PREEZ, CC. 2006. *Soil Survey: Mkabela Catchment*. Department of Soil, Crop and Climate Sciences University of the Free State, Bloemfontein

LORENTZ, S.A., AND SCHULZE, R.E. 1995. Sediment Yield. In: Schulze, R.E. Hydrology and Agrohydrology: A Text to Accompany the ACRU 3.00 Agrohydrological Modelling System. *Water Research Commission, Pretoria, Report TT69/95*. pp AT16-1 to AT16-34.

LORENTZ S, BERRY S, AND ROSSOUW N. 2006. Field to Catchment Scale Modelling of Selected NPS Pollutants. *Workshop on: Diffuse Pollution and Its Role in the Management of Water Quality in South Africa.* WISA Biennial Conference and Exhibition, Durban, May 2006.

LORENTZ SA, KOLLONGEI J, SNYMAN N, BERRY SR, JACKSON W, NGALEKA K, PRETORIUS JJ, CLARK D and THORNTON-DIBB S (2012). *Modelling Nutrient and Sediment Dynamics at the Catchment Scale.* WRC Report No. 1516/3/12, Water Research Commission, Pretoria

SCHULZE, R.E. 1995. *Hydrology and Agrohydrology: A Text to Accompany the ACRU 3.00 Agrohydrological Modelling System*. Water Research Commission, Pretoria, Report TT69/95. pp AT16-1 to AT16-34.

SHARPLEY AN AND WILLIAMS JR (ed). 1990. *EPIC-Erosion/productivity impact calculator: Model documentation*. USDA-ARS, Tech Bulletin No 1768. 235pp. (1990).

SOIL CLASSIFICATION WORKING GROUP (1991) *Soil Classification. A Taxonomic System for South Africa*. Dept. of Agricultural Development, Pretoria, South Africa.

Team: Economics of Agricultural NPS Pollution Management

ARROW, KJ and DEBREU, G. 1954. Existence of an equilibrium for a competitive economy. *Econometrica*, 22: 265-290.

JOHANSSON, RC, GOWDA, PH, MULLA DJ and DALZELL BJ. 2004. Metamodelling phosphorus best management practices for policy use: a frontier approach. *Agricultural Economics*, 30: 63-74.

JUST, RE and POPE, RD. 1979. Production function estimation and related risk considerations. *American Journal of Agricultural Economics*, 61(2):276-284.

MATTHEWS N and GROVÉ B (2012). *Modelling Economic-Environmental Trade-Offs of Agricultural Non-Point Source Pollution Control Measures*. WRC Report No. 1516/4/12, Water Research Commission, Pretoria.

RASMUSSEN, S. 2004. Optimising production under uncertainty: Generalisation of the state-contingent approach and comparison of methods for empirical application. *Unit of Economics Working Paper 2004/2*. The Royal Veterinary and Agricultural University

RASMUSSEN, S and KARANTININIS, K. 2005. Estimating state-contingent production functions. Paper presented at the *XIth Congress of the European Association of Agricultural Economists (EAAE)*. Copenhagen, Denmark.

RICHARDSON, JW, KLOSE, SL and GRAY, AW. 2000. An applied procedure for estimating and simulating multivariate empirical (MVE) probability distributions in farm-level risk assessment and policy analysis. *Journal of Agricultural and Applied Economics*, 32(2):299-318.

TEAGUE, ML, BERNARDO, DJ and MAPP, HP. 1995. Meeting environmental goals efficiently on a farm-level basis. *Review of Agricultural Economics*, 17:37-50.

STOORVOGEL, JJ, ANTLE, JM, CRISSMAN, CC and BOWEN, W. 2001. *The Tradeoff Analysis Model Version 3.1: A Policy Decision Support System for Agriculture (User Guide)*. Laboratory of Soil Science and Geology, Wageningen University, The Netherlands.

USDA SOIL CONSERVATION SERVICE (1983) *National Engineering Handbook Section 4 Hydrology*, Chapter 19.

APPENDIX A: JOURNAL/CONFERENCE PAPERS PRODUCED DURING PROJECT

ANNANDALE JG, STEYN JM, BÉNADE N and VAN DER LAAN M. (2008). The Soil Water Balance (SWB) project: What have we achieved and where are we going? *Proceedings of the SANCID Symposium,* Club Mykonos, Langebaan, 18-20 November 2008.

GÖRGENS A, GROVÉ B, ANNANDALE J, LORENTZ S, JOVANOVICH N, DU PREEZ C, MATTHEWS N, VAN DER LAAN M, LE ROUX J and LYONS S (2011). Agricultural non-point source pollution: modelling and economics. *Presentation at the Water Research Commission's 40th Anniversary Celebration Conference*, Emperor's Palace, August 2011.

JOVANOVIC NZ and PETERSEN C (2009). An Excel-based index (PestEX) for environmental mobility of pesticides in relation to water resources. In: C.A. Brebbia, N. Jovanovic, E. Tiezzi (eds.) *Management of Natural Resources, Sustainable Development and Ecological Hazards II*, 415-426. ISBN 978-1-84564-204-4, Wit Press, Southampton, UK.

JOVANOVIC NZ, BUGAN RDH, PETERSEN C, DE CLERCQ WO, ROZANOV A and BOTHA H (2010). Generation and size distribution of sediment eroded in a small-scale catchment of the Western Cape (South Africa). In: A.M. Marinov, C.A. Brebbia (eds.) *Water Pollution X*, 195-206. ISBN 978-1-84564-448-2, Wit Press, Southampton, UK.

MATTHEWS, N., GROVÉ, B., BARNARD, J.H. and VAN RENSBURG, L.D. (2008). An economic case for salinity management. *3rd South African National Commission on Irrigation and Drainage Symposium,* Langebaan, 18-20 November 2008.

MATTHEWS, N., GROVÉ, B., BARNARD, J.H. and VAN RENSBURG, L.D. (2008). Economic analysis of salinity management. *1st Annual Orange River Basin Symposium, Bloemfontein*, 12-14 November 2008.

MATTHEWS, N., GROVÉ, B., BARNARD, J.H. and VAN RENSBURG, L.D. (2008). Modelling the economic effects of irrigation water salinity management for sustainable crop production. *46th Annual Conference of the Agricultural Economics Association of South Africa*, Windhoek, Namibia, 23-26 September 2008.

VAN DER LAAN M, ANNANDALE JG, DU PREEZ CC, TESFAMARIAM E, BÉNADE N, BRISTOW KL and STIRZAKER RJ. (2008). A new capability in SWB-Sci to model nitrogen and phosphorus dynamics in cropping systems. *Proceedings of the SANCID Symposium*, Club Mykonos, Langebaan, 18-20 November 2008.

VAN DER LAAN, M; ANNANDALE, JG; DU PREEZ, CC and LORENTZ, SL (2009). Obtaining the parameters required to model labile P for South African soils. *South African Journal of Plant and Soil*, 26, 213-219.

VAN DER LAAN, M; STIRZAKER, RJ; ANNANDALE, JG; BRISTOW, KL and DU PREEZ, CC (2010). Monitoring and modelling draining and resident soil water nitrate concentrations to estimate leaching losses. *Agricultural Water Management*, 97, 1779-1786.

VAN DER LAAN, M; STIRZAKER, RJ; ANNANDALE, JG; BRISTOW, KL and DU PREEZ, CC (2010). Interpretation of electrical conductivity measurements from ceramic suction cups, wetting front detectors and capacitance sensors. *South African Journal of Plant and Soil*, submitted.

VAN DER LAAN, M; STIRZAKER, RJ; ANNANDALE, JG; BRISTOW, KL and DU PREEZ, CC (2010). Estimating nitrate leaching losses through the monitoring and modelling of mobile and resident soil water concentrations. *One Water Many Futures Irrigation Australia Conference*, Sydney, June 2010.

VAN DER LAAN, M; BRISTOW, KL; STIRZAKER, RJ; ANNANDALE, JG and DU PREEZ, CC (2010). Linking measurement and modelling more closely to improve estimates of solute leaching losses. *ICID Working Group on the Environment 'Nutrient leaching from agricultural soils' workshop*. Yogyakarta, Indonesia, October 2010.

VAN DER LAAN, M; STIRZAKER, RJ; ANNANDALE, JG; BRISTOW, KL and DU PREEZ, CC (2010). Estimating leaching losses from mobile and immobile soil water nitrate concentrations. *Combined Congress*, Bloemfontein, 19-21 January 2010.

APPENDIX B: POST-GRADUATE STUDENTS SUPPORTED DURING PROJECT

Name	Gender	Population Group	Degree	University	Country Of Origin
Berry S	Male	White	MSc	University of KwaZulu-Natal	RSA
Bester C	Male	White	MSc	University of KwaZulu-Natal	RSA
Frantz G	Male	Coloured	MSc	University of the Western Cape	RSA
Harun I	Male	Coloured	MSc	University of the Western Cape	RSA
Kollongei J	Male	African	PhD	University of KwaZulu-Natal	Kenya
Le Roux J	Male	White	PhD	University of Pretoria	RSA
Matthews N	Female	White	PhD	University of the Free State	RSA
Ngaleka K	Male	African	MSc	University of the Free State	Dem. Rep. Congo
Ojo O	Female	African	MSc	University of the Western Cape	Nigeria
Phahlane O	Male	African	MSc	University of the Free State	RSA
Titshall L	Male	White	Post-Doc	University of KwaZulu-Natal	RSA
Van der Laan M	Male	White	PhD	University of Pretoria	RSA
Zondi N	Male	African	Honours	University of KwaZulu-Natal	RSA