



Bio-inspired Optimization in Integrated River Basin Management

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Abstract

Water resources worldwide are facing severe challenges in terms of quality and quantity. It is essential to conserve, manage, and optimize water resources and their quality through integrated water resources management (IWRM). IWRM is an interdisciplinary field that works on multiple levels to maximize the socio-economic and ecological benefits of water resources. Since this is directly influenced by the river's ecological health, the point of interest should start at the basin-level. The main objective of this study is to evaluate the application of bio-inspired optimization techniques in integrated river basin management (IRBM). This study demonstrates the application of versatile, flexible and yet simple metaheuristic bio-inspired algorithms in IRBM.

In a novel approach, bio-inspired optimization algorithms Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO) are used to spatially distribute mitigation measures within a basin to reduce long-term annual mean total nitrogen (TN) concentration at the outlet of the basin. The Upper Fuhse river basin developed in the hydrological model, Hydrological Predictions for the Environment (HYPE), is used as a case study. ACO and PSO are coupled with the HYPE model to distribute a set of measures and compute the resulting TN reduction. The algorithms spatially distribute nine crop and subbasin-level mitigation measures under four categories. Both algorithms can successfully yield a discrete combination of measures to reduce long-term annual mean TN concentration. They achieved an 18.65% reduction, and their performance was on par with each other. This study has established the applicability of these bio-inspired optimization algorithms in successfully distributing the TN mitigation measures within the river basin.

Stakeholder involvement is a crucial aspect of IRBM. It ensures that researchers and policymakers are aware of the ground reality through large amounts of information collected from the stakeholder. Including stakeholders in policy planning and decision-making legitimizes the decisions and eases their implementation. Therefore, a socio-hydrological framework is developed and tested in the Larqui river basin, Chile, based on a field survey to explore the conditions under which the farmers would implement or extend the width of vegetative filter strips (VFS) to prevent soil erosion. The framework consists of a behavioral, social model (extended Theory of Planned Behavior, TPB) and an agent-based model (developed in NetLogo) coupled with the results from the vegetative filter model (Vegetative Filter Strip Modeling System, VFSSMOD-W). The results showed that the ABM corroborates with the survey results and the farmers are willing to extend

the width of VFS as long as their utility stays positive. This framework can be used to develop tailor-made policies for river basins based on the conditions of the river basins and the stakeholders' requirements to motivate them to adopt sustainable practices.

It is vital to assess whether the proposed management plans achieve the expected results for the river basin and if the stakeholders will accept and implement them. The assessment via simulation tools ensures effective implementation and realization of the target stipulated by the decision-makers. In this regard, this dissertation introduces the application of bio-inspired optimization techniques in the field of IRBM. The successful discrete combinatorial optimization in terms of the spatial distribution of mitigation measures by ACO and PSO and the novel socio-hydrological framework using ABM prove the forte and diverse applicability of bio-inspired optimization algorithms.

Keywords: river basin management, bio-inspired algorithms, parameter optimization, spatial distribution, socio-hydrology

Zusammenfassung

Die Wasserressourcen stehen weltweit vor großen Herausforderungen in Bezug auf Qualität und Quantität. Die Erhaltung, Bewirtschaftung und Optimierung der Wasserressourcen und ihrer Qualität durch integriertes Wasserressourcenmanagement (IWRM) ist von entscheidender Bedeutung. IWRM ist ein interdisziplinärer Wissenschaftsbereich, der mehrere Ebenen einbezieht, um den sozioökonomischen und ökologischen Nutzen der Wasserressourcen zu maximieren. Da dies direkt von der ökologischen Gesundheit des Flusses abhängt, sollte das Interesse auf der Ebene des Einzugsgebiets beginnen. Diese Studie demonstriert die Anwendung vielseitiger, flexibler und dennoch einfacher metaheuristischer bioinspirierter Algorithmen im IRBM. Das Hauptziel dieser Studie ist es, die Anwendung von bioinspirierten Optimierungstechniken im integrierten Flussgebietsmanagement (IRBM) auszuwerten.

In einem neuartigen Ansatz werden die bioinspirierten Optimierungsalgorithmen Ant Colony Optimization (ACO) und Particle Swarm Optimization (PSO) eingesetzt, um Maßnahmen in einem Einzugsgebiet räumlich zu verteilen und so die langfristige mittlere jährliche Gesamtstickstoff (TN)-Konzentration am Ausgang des Einzugsgebiets zu verringern. Das Einzugsgebiet der Oberen Fuhse, das mit dem hydrologischen Modell Hydrological Predictions for the Environment (HYPE) entwickelt wurde, wird als Fallstudie verwendet. ACO und PSO werden mit dem HYPE-Modell gekoppelt, um die ausgewählten Maßnahmen zu verteilen und die daraus resultierende TN-Reduktion zu berechnen. Die Algorithmen verteilen neun Minderungsmaßnahmen auf Ebene der Kulturen und Teileinzugsgebiete unter vier Kategorien räumlich. Beide Algorithmen können erfolgreich eine diskrete Kombination von Maßnahmen zur Verringerung der langfristigen mittleren jährlichen TN-Konzentration liefern. Sie erreichten eine Reduktion von 18,65 % und ihre Leistung war gleichwertig. Diese Studie hat die Anwendbarkeit dieser bioinspirierten Optimierungsalgorithmen bei der erfolgreichen Verteilung der Minderungsmaßnahmen innerhalb des Flusseinzugsgebiets nachgewiesen.

Die Einbeziehung von Interessengruppen ist ein entscheidender Aspekt des IRBM. Sie stellt sicher, dass Forscher und politische Entscheidungsträger die Realität vor Ort kennen, indem sie eine große Menge an Informationen von den Interessenvertretern einholen. Die Einbeziehung von Interessengruppen in die politische Planung und Entscheidungsfindung legitimiert die Entscheidungen und erleichtert ihre Umsetzung. Daher wurde ein soziohydrologischer

Framework entwickelt und im Einzugsgebiet des Larqui, Chile, getestet, um die Bedingungen zu untersuchen, unter denen die Landwirte Gewässerrandstreifen (vegetative Filterstreifen, VFS) zur Verhinderung der Bodenerosion anlegen oder ausweiten würden. Der Rahmen besteht aus einem sozialen Verhaltensmodell (erweiterte Theory of Planned Behavior, TPB) und einem agentenbasierten Modell (entwickelt in NetLogo), das mit den Ergebnissen des vegetativen Filtermodells (Vegetative Filter Strip Modeling System, VFSSMOD-W) gekoppelt ist. Die Ergebnisse zeigten, dass das ABM mit den Umfrageergebnissen übereinstimmt und die Landwirte bereit sind, die Breite des VFS zu vergrößern, solange ihr Gewinn positiv bleibt. Dieser Rahmen kann genutzt werden, um maßgeschneiderte Strategien für Flusseinzugsgebiete zu entwickeln, die auf den Bedingungen der Flusseinzugsgebiete und den Anforderungen der Interessengruppen basieren, um sie zu motivieren, nachhaltige Praktiken anzuwenden.

Es ist von entscheidender Bedeutung zu beurteilen, ob die vorgeschlagenen Bewirtschaftungspläne die erwarteten Ergebnisse für das Flusseinzugsgebiet erzielen und ob die Beteiligten sie akzeptieren und umsetzen werden. Die Bewertung mit Hilfe von Simulationswerkzeugen gewährleistet eine effektive Umsetzung und Verwirklichung der von den Entscheidungsträgern festgelegten Ziele. In diesem Zusammenhang wird in dieser Dissertation die Anwendung von bioinspirierten Optimierungstechniken im Bereich des IRBM vorgestellt. Die erfolgreiche diskrete kombinatorische Optimierung in Bezug auf die räumliche Verteilung von Minderungsmaßnahmen durch ACO und PSO und der neuartige sozio-hydrologische Rahmen unter Verwendung von ABM beweisen die Stärke und vielfältige Anwendbarkeit von bioinspirierten Optimierungsalgorithmen.

Stichworte: *Flussgebietsmanagement, bioinspirierte Algorithmen, Parameteroptimierung, räumliche Verteilung, Sozio-Hydrologie*

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Contents

| | |
|--|-----------|
| 1. Motivation and Objectives | 1 |
| 1.1 Background | 1 |
| 1.2 Motivation and Objectives | 6 |
| 1.3 Thesis Structure and Overview | 7 |
| 2. State of Art | 8 |
| 2.1 Optimization..... | 8 |
| 2.2 Metaheuristics Optimization | 9 |
| 2.3 Bio-inspired Optimization..... | 12 |
| 2.3.1 Swarm Intelligence (SI) based algorithms..... | 12 |
| 2.3.2 Non-SI-based algorithms..... | 22 |
| 2.4 Agent-based model (ABM)..... | 25 |
| 3. Spatial distribution of mitigation measures to reduce total nitrogen concentration using Ant Colony Optimization and Particle Swarm Optimization | 27 |
| 3.1 Introduction | 28 |
| 3.2 Materials and Methods | 32 |
| 3.2.1 Study Area | 32 |
| 3.2.2 Ant Colony Optimization (ACO) | 35 |
| 3.2.3 Particle Swarm Optimization (PSO)..... | 39 |
| 3.3 Results and Discussion..... | 42 |
| 3.3.1 Parameter selection..... | 42 |
| 3.3.2 Spatial distribution of mitigation measures | 42 |
| 3.4 Conclusions | 50 |
| 4. Application of the theory of planned behavior with agent-based modeling for sustainable management of vegetative filter strips..... | 52 |
| 4.1. Introduction | 53 |
| 4.2. Materials and methods | 56 |

| | |
|---|------------|
| 4.2.1. Study area | 56 |
| 4.2.2. Modeling framework | 57 |
| 4.3. Results and Discussion..... | 66 |
| 4.3.1 Statistical analysis of the field survey and the theoretical model..... | 66 |
| 4.3.2 VFSSMOD-W Modeling | 70 |
| 4.3.3 ABM Modeling..... | 71 |
| 4.4 Conclusions | 74 |
| 5. Conclusions and Outlook | 77 |
| 6. Bibliography | 82 |
| Appendix A | 132 |
| Appendix B | 136 |
| Appendix C | 138 |

List of Tables

| | |
|---|-----|
| Table 3.1 Mitigation measures to reduce TN and their level of implementation in HYPE..... | 345 |
| Table 3.2 Parameter selection for ACO and PSO..... | 42 |
| Table 3.3 Measures selected by ACO and PSO..... | 43 |
| Table 4.1 Parameters of the utility function..... | 63 |
| Table 4.2 Decision-making rules for different types of agents..... | 64 |
| Table 4.3 VIF, outer loading, t and p-value of constructs | 68 |
| Table 4.4 Agent decision depending on the behavioral categorization | 73 |

List of Figures

| | |
|---|----|
| Figure 2.1 Classification of optimization techniques | 9 |
| Figure 2.2 Disciplines inspiring metaheuristic algorithms | 10 |
| Figure 2.3 Chronology of various bio-inspired optimization techniques developed..... | 15 |
| Figure 3.1 Upper Fuhse river basin, Germany..... | 32 |
| Figure 3.2 Flowchart of Ant Colony Optimization for spatial distribution of measures | 38 |
| Figure 3.3 Flowchart of Particle Swarm Optimization for spatial distribution of measures | 41 |
| Figure 3.4 Selection of crop-level measures by ACO | 44 |
| Figure 3.5 Selection of crop-level measures by PSO | 45 |
| Figure 3.6 Annual mean TN achieved by ACO and PSO..... | 46 |
| Figure 3.7 Long-term annual mean percentage reduction of TN by ACO | 47 |
| Figure 3.8 Long-term annual mean percentage reduction of TN by PSO | 48 |
| Figure 3.9 Performance indicator map..... | 49 |
| Figure 4.1 Schematic representation of the workflow | 58 |
| Figure 4.2 Extended Theory of Planned Behavior model..... | 60 |
| Figure 4.3 Formative-formative type model of the extended TPB..... | 67 |
| Figure 4.4 Simplified higher-order formative-formative type PLS-SEM model of extended TPB results | 69 |
| Figure 4.5 Performance efficiency of different widths of VFS in soil retention for all classes combined together..... | 71 |
| Figure 4.6 Decision of the agents on the width of VFS at the end of every three years..... | 72 |

Abbreviations

ABC – Artificial Bee Colony

ABM – Agent-Based Modelling

ACO – Ant Colony Optimization

ANN – Artificial Neural Network

BCO – Bacterial Foraging Optimization

BfG – German Federal Institute of Hydrology

BMP – Best Management Plans

CS – Cuckoo Search

DE – Differential Evolution

DEMC – Differential Evolution Markov Chain

DP – Dynamic Programming

EA – Evolutionary Algorithms

EP – Evolutionary Programming

ES – Evolutionary Strategies

EU – European Union

FA – Firefly Algorithm

FD – Flood Directive

GA – Genetic Algorithm

GP – Genetic Programming

GWO – Grey Wolf Optimizer

HYPE – Hydrological Predictions for the Environment

IRBM – Integrated River Basin Management

IWRM – Integrated Water Resources Management

LP – Linear Programming

NLP – Non-Linear Programming

PSO – Particle Swarm Optimization

RBD – River Basin Districts

RBMP – River Basin Management Plan

SEM – Structural Equation Modeling

SI – Swarm-Intelligence

STP – Sewage Treatment Plant

TN – Total Nitrogen

TPB – Theory of Planned Behavior

VFS – Vegetative Filter Strips

WFD – Water Framework Directive

1. Motivation and Objectives

1.1 Background

Water is a vital resource encompassing hydrological, ecological, social and economic dimensions. Effective management of such a vital resource directly and significantly benefits ecology, communities, and regions. Humans rely on water for survival, yet water resources worldwide face threats from overuse, contamination, disruption of flows and a changing climate. Though natural resources management has been in practice, albeit in different forms, since the earliest periods of human settlement, the focus on river basin management (RBM) came about only in the last century (Hooper, 2005). This is due to the acceptance of the significance of water as an essential resource for human existence and ecosystem functioning (MacKenzie, 1996). In the early twentieth century, RBM focused on the ethics of resource exploitation to achieve economic development.

In contrast, later in the century, it shifted to resource conservation and sustainable resource management. The shift happened for two critical reasons, as outlined by Hooper (2005). First, the conventional approach was a reactive, fragmented approach without understanding the inter-relationships between resource management and issues with ecological functions. Second, the inter-dependencies of biological, economic, and human systems were ignored and addressed separately, leading to competing management goals. The concept Integrated Water Resource Management (IWRM) was officially articulated in the 1992 Dublin Conference on Water and Environment and the 1992 United Nations Rio Summit on Environment and Development (Mukhtarov, 2008). One of the primeval attempts of IWRM implementation, even before the term was introduced, was in 1933 by the Tennessee Valley Authority (TVA). To control floods and produce power, TAV constructed dams. And in its evaluation, TAV included the assessment of erosion control, recreation, public health and welfare.

Global Water Partnership defines IWRM as a process that “*promotes the coordinated development and management of water, land and related resources in order to maximize economic and social welfare in an equitable manner without compromising the sustainability of vital ecosystems and the environment*” (GWP, 2000). The primary components of IWRM include

managing water resources at the lowest level, optimizing supply and managing demand, providing equitable access to water resources through participatory and transparent governance, developing improved and integrated policy, establishing regulatory and institutional frameworks, and ensuring an inter-sectoral approach to decision-making. In most parts of the world, the river is a crucial water resource as it is a hydrological conduit that receives excess water from precipitation through runoff, infiltration and groundwater movement. The ecological health of the land systems and urban settlements is directly dependent on the river's ecological health (Hooper, 2005). Therefore, it is apt to consider a river basin as a natural unit for decision-making.

IWRM is best implemented at the river basin level using an Integrated River Basin Management (IRBM) approach. IRBM emphasizes interdisciplinary coordination, planning and management of water resources, sustainable development and strategies for water, land and other related resources in a river basin to achieve long-term sustainability (Downs et al., 1991; Savenije and Van der Zaag, 2008; Bandaragoda and Babel 2010). IRBM is, therefore, a subset of IWRM (Elfithri and Mokhtar, 2018). IRBM aims to develop and implement a holistic framework of assessment, planning, decision-making, coordination, and policy development with active stakeholder involvement (Mostert et al., 2007). By using the expertise of the scientific community, the good governance of the decision-making body, and valuable inputs from the stakeholders, a balanced approach to water resource management is achieved. IRBM identifies the community's best river management practices with respect to land use management, agriculture, economics, urban planning, etc. In addition, it prioritizes the river's health, which is beneficial to the ecosystems, communities, economies, and biological processes within it. A crucial output of a system of IRBM is the development of plans in which water quantity, quality, and environmental integrity are integrated at the highest level (Jaspers, 2003).

Effective implementation of IRBM can alleviate the communities from poverty, help prepare the communities against the disasters caused by extreme events, provide perennial water sources, and achieve sustainable development with healthy ecosystems. Though the concept of IRBM is clear and widely accepted, its practical application is challenging. To ensure sustainable river basin development, it is pertinent to address the interests of various actors within the basin and plan for demands at different scales. This is often not considered in IRBM. One should also take into consideration the topographical and resource limitations. These issues can be addressed

from a systems viewpoint by prioritizing the relationship between the system components rather than addressing them separately (Ravesteijn et al., 2009).

Another impediment faced during the practical application of IRBM is the implementation of management plans. In many cases, it is attributed to institutional factors (Watson, 2004). This can be overcome by opting for collaborative approaches to solve problems by involving all stakeholders during the decision-making process. For effective IRBM, institutions must be flexible and adaptable in order to respond tactfully to changes in knowledge, circumstances and needs of the stakeholders. The success of IRBM depends on the institutional alliance and the ability of participants to reach a consensus through effective negotiation.

IRBM has been made prominent in the European Union (EU) by two directives — the Floods Directive (FD, 2007/60/EC) in 2007 and the Water Framework Directive (WFD, 2000/60/EC) in 2000 (Evers, 2016). WFD is by far the most comprehensive environmental legislation that consolidates the previous water legislation and extends to include the concepts of river basin management to entire European Union. According to WFD, the Member States must identify and assign water bodies to River Basin Districts (RBD) based on hydrological basins (with coastal and ground waters assigned to the most appropriate District). Furthermore, a competent authority is assigned to each RBD to coordinate the implementation of the Directive within the RBD. The competent authority is responsible for identifying critical water management issues and for the development of the River Basin Management Plan (RBMP) for that basin (Griffiths, 2002). The RBMP provides a detailed account of how the objectives of WFD (ecological status, quantitative status, chemical status, and protected area objectives) will be achieved for the river basin within the given period. The EU Member States must achieve ‘good status’ in all surface water and groundwater bodies by 2015 and 2027, respectively, at the latest. The plan includes an analysis of river basin characteristics, anthropogenic impacts on the status of waters in the basin, evaluation of the influence of the existing legislation and identification of the ‘gap’ to meet the set-out objectives, strategies to fill the gap, and evaluation of the cost-effectiveness of the measures.

Such analysis is performed using modelling systems to quantify the nutrient loads and interactions in the river basin. Over the years, many models have been developed, coupling the concepts of hydrology and crop growth to understand nitrogen dynamics in basins. Some of these

models include but are not limited to Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS, Kinsel, 1980), Generalized Watershed Loading Function (GWLF, Haith and Shoemaker, 1987), SOIL Nitrogen model (SOILN, Johnsson et al., 1987), DeNitrification DeComposition (DNDC, Li et al., 1992), Leaching Estimation and CHemistry model N version (LEACHN, Hutson and Wagenet 1992); Water and Agrochemicals in the soil and Vadose Environment (WAVE, Vanclooster et al., 1995), Soil and Water Assessment Tool (SWAT, Arnold et al., 1998), Soil and Water Integrated Model (SWIM, Krysanova et al., 1998), Watershed Analysis Risk Management Framework (WARMF, Herr and Chen, 2012), Hydrological Simulation Program – Fortran (HSPF, Duda et al., 2012), MIKE Système Hydrologique Européen (MIKE-SHE, Jaber and Shukla, 2012) and Hydrological Predictions for the Environment model (HYPE, Lindström et al., 2010). A detailed review of different models used is given by Bouraoui and Grizzetti (2013). These models require a large amount of observed data sets and must be calibrated. An alternative to the physical-based models is the use of artificial neural networks (ANN) to simulate and predict nitrogen concentration in river basins (Suen and Eheart, 2003).

According to Lek et al. (1999), ANN can assimilate the knowledge about the relationship between basin characteristics and nitrogen levels in river reaches and, therefore, predict the concentration levels. They developed an ANN approach and tested it on 927 tributary sites. Kim et al. (2012) used multilayered ANN to predict the pollutant load from the West Branch Delaware River basin and compared it with two hydrological models, GWLF and SWAT. The feed-forward ANN could predict pollutant load better than the two hydrological models. Suen and Eheart (2003) compared the abilities of back-propagation neural networks and radial basis function neural networks against SWAT to model water quality with a focus on nitrate concentrations. Their results indicated that both neural networks perform better than SWAT, and radial basis function neural networks achieve the best results. Kim and Gilley (2008) used ANN to estimate the soil erosion and nutrient concentration from croplands successfully. Wagh et al. (2017) used a back propagated ANN to predict groundwater quality and tested it on 40 sampling sites in the Kadava river basin for nitrate pollution. A satisfactory fit was obtained for the ANN results against the experimental data obtained from sampling sites. They concluded that with the proposed ANN, groundwater resources could be better managed. These models can be coupled with decision

support systems to provide insight into the critical aspects of decision-making and run various scenarios to analyze what works best for the given basin.

A river system faces many uncertainties, such as variability in water availability, technological advancements, fluctuations in demand, and complex interdependent processes like pollution from point and non-point sources, surface runoff, storm runoff, water reuse and recycle etc. These uncertainties pose a tremendous challenge for water management and can be addressed by optimization. Optimization refers to the process of effective use of a resource under the given circumstances or constraints. In the early 1960s, the use of optimization in water resources planning and management started with linear and dynamic programming (Tayfur, 2017). Some of the applications of these methods include reservoir operation and management (Faber and Stedinger, 2001), flood control (Needham et al., 2000), water allocation optimization for conflicting demands (Meng et al., 2018), optimal pump scheduling (Nace et al. 2001; Pasha and Lansley 2009; Chiu et al., 2010), water supply system (Hsu and Cheng, 2002), multi-reservoir modeling (Chandramouli and Raman 2001), and hydropower reservoir operation (Yoo, 2009; Zhao et al. 2014). The application of conventional optimization techniques in water resources management has been reviewed by Singh (2012). Although classical mathematical optimization techniques can solve water resources management problems, they have a specific formulation requirement for defining the problem, objective function, and constraints. To do this, users will have to simplify the formulation of complex water resource management problems, which could introduce system discrepancies (Horne et al., 2016).

With the advancement in computational sciences in the last few decades, many intelligent optimization algorithms have been developed for data processing, planning, and decision-making. In the last decade, bio-inspired optimization has been widely applied to solve problems across multiple fields like vehicle routing, traffic management, operation scheduling, and sustainable energy management (Darwish, 2018). In water resource management, these algorithms have been applied to flood control and mitigation, reservoir operation, irrigation, flood routing, parameter optimization of rainfall-runoff processes, sediment transport, groundwater management, water quality monitoring, and land-use allocation. State of the art on bio-inspired optimization techniques is discussed/ provided in Chapter 2.

1.2 Motivation and Objectives

This research aims to demonstrate the ability of different bio-inspired optimization algorithms for various aspects of IRBM. It intends to encourage other researchers to utilize the available well-established bio-inspired optimization techniques in the field of IRBM. In this thesis, bio-inspired optimization techniques have been applied to two different aspects of IRBM. The objectives of this research are as follows:

First, *to spatially distribute the mitigation measures in a river basin using bio-inspired optimization*. Though bio-inspired algorithms have been used for land-use allocation, this research is the first time to use them in mitigation measures distribution. Two bio-inspired optimization algorithms, Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO), are used to spatially distribute mitigation measures to reduce long-term annual mean total nitrogen (TN) concentration to achieve maximum reduction. According to the Lower Saxony water body monitoring system (GÜN), 63% of measuring stations in Germany recorded TN concentrations greater than 2.8 mg/l. The Peine gauging station located at the upper Fuhse river basin outlet is one of them and, therefore, used as a case study in this research.

Second, *to develop a socio-hydrological framework in order to evaluate the perspective of stakeholders (farmers) on implementing a mitigation measure in a river basin*. The essential aspect of IRBM is collaboration to ensure that the environmental policies developed are tailored to improve the environmental status while optimizing the stakeholders' and their economic interests. Valuable information, knowledge, or practical resources outside the realms of scientists and managers are vital to enable problems to be defined clearly, propose alternatives or management options, and assess the potential policies that best fit the circumstances. Through agent-based modelling (ABM), one could model the behavior of actors within the basin in order to find optimum solutions. A case study is conducted with farmers from the Larqui river basin, Chile, to understand their standpoint on the use of vegetative filter strips as a measure to reduce soil loss in their agricultural fields and protect water bodies. An ABM is developed using the behavioral categorization derived from an on-site survey of the farmers, related decision rules, and utility functions of agricultural activities.

1.3 Thesis Structure and Overview

This thesis highlights the application of bio-inspired optimization techniques in different aspects of IRBM. Chapters 3 and 4 are scientifically complete by themselves, consisting of the introduction, state of art, methodology, and result and discussions corresponding to the objectives described. These chapters are under one umbrella; however, the results of each chapter stand-alone. Chapter 3 will be submitted to a journal as a scientific article, and Chapter 4 has already been published by the researcher as a first author during her Ph.D. period. This thesis is structured as follows:

1. Chapter 1 describes the motivation behind this study and explains the two objectives involved.
2. Chapter 2 provides an overview of the state of art in the field of bio-inspired optimization in integrated river basin management.
3. Chapter 3 introduces the novel application of two bio-inspired algorithms, Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO), to spatially distribute mitigation measures to reduce TN concentration in the river basin.
4. Chapter 4 presents an innovative socio-hydrological modeling framework for developing environmental policies using agent-based modelling. A behavior model is developed based on a modified Theory of Planned Behavior (TPB) (published as Kasargodu Anebagilu, P., Dietrich, J., Prado-Stuardo, L., Morales, B., Winter, E., and Arumi, J. L, (2021). Application of the theory of planned behavior with agent-based modeling for sustainable management of vegetative filter strips, *Journal of Environmental Management*, 284, 112014, ISSN 0301-4797. <https://doi.org/10.1016/j.jenvman.2021.112014>).
For the fulfillment of this objective, the author contributed to the conceptualization, survey analysis, modelling, coding, writing and revising of the manuscript.
5. Chapter 5 is the final chapter that provides the synopsis of the results obtained and presents the main findings from the three research objectives. It also summarizes the future research propositions that could be considered while using bio-inspired optimization for IRBM and the area in which more research is required in the near future.

2. State of Art

2.1 Optimization

Optimization techniques are used by people worldwide to solve problems and select the best option under the given circumstances from many available options. Until the late 1980s, classical mathematical techniques (deterministic) were successfully used in engineering, planning, and management. These include linear (LP, Kantorovich, 1939), nonlinear (NLP) and dynamic programming (DP). However, when they were used to solve complex problems with large-scale combinatorial and highly nonlinear optimization, these techniques exhibited poor performance (Memmah et al., 2015; Silveira et al., 2021). The poor performance has been attributed to the limitations of conventional optimization techniques in dealing with the following two aspects:

1) Nonlinear objectives and constraints: mathematical techniques have predefined objectives and constraints formulation. However, complex problems like those in IRBM often have numerous nonlinear objectives and constraints, which will have to be simplified to fit the formulation, thus, adding bias to the optimization process;

2) Many variables: mathematical techniques struggle to deal with problems with many variables. As the search space's dimensionality increases exponentially with the number of variables, the techniques cannot perform an exhaustive search within a reasonable time (Memmah et al., 2015; Kumar and Yadav, 2022).

In this regard, stochastic approaches are considered more flexible and efficient in solving large and complex optimization problems. Two main stochastic approaches were developed in the late 1970s to overcome the limitations of deterministic optimization techniques: heuristic and metaheuristic optimization (Rao and Keesari, 2018). While a heuristic algorithm is aimed to solve a problem faster, it does not guarantee a global optimal solution. However, to solve a complex problem in a reasonable computational time, a heuristic algorithm is better than an impractical exhaustive search (Sörensen, 2013). Classification of the optimization techniques is shown in Figure 2.1.

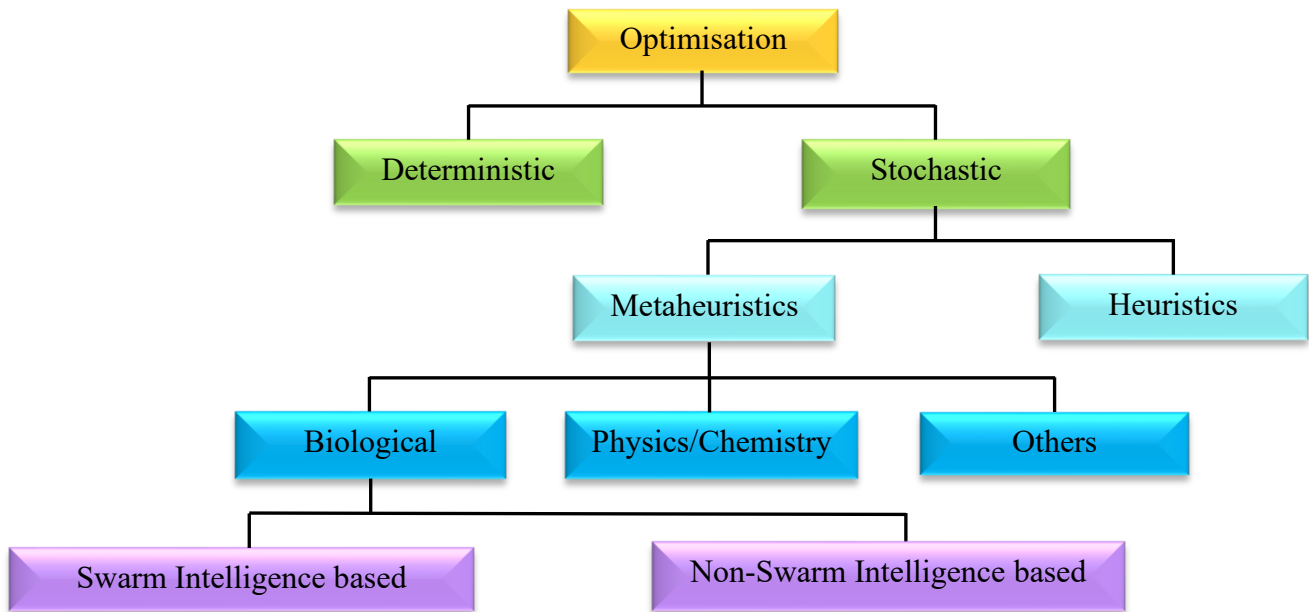


Figure 2.1 Classification of optimization techniques

2.2 Metaheuristics Optimization

The term metaheuristic was coined by Glover (1986), and Sörensen and Glover (2013) defined metaheuristics as ‘*a high-level problem-independent algorithmic framework that provides a set of guidelines or strategies to develop heuristic optimization algorithms. The term is also used to refer to a problem-specific implementation of a heuristic optimization algorithm according to the guidelines expressed in such a framework*’. It is a higher-level adaptive computing technique that provides a ‘sufficiently good solution’ to an optimization problem offering a better trade-off in terms of computational time and solution quality. The critical point to achieving this is finding the perfect balance between exploration and exploitation. Exploration distinguishes the most promising regions in a search space where the optimal solution could be positioned; exploitation amplifies local search in the identified region.

The use of metaheuristic algorithms started in the 1980s with Simulated Annealing (Kirkpatrick, 1983) and Tabu Search (Glover, 1989). Research in metaheuristic algorithms started to thrive in the 1990s due to the successful widespread applications of algorithms like genetic and swarm intelligence-based algorithms. Since then, more than hundreds of metaheuristic algorithms have been developed inspired by various disciplines of science and everyday activities. In spite of

the extensive research in the field of metaheuristics, Sörensen et al. (2017) estimate that the field of metaheuristics hasn't reached maturity, and there is still a long road ahead. Though a large percentage of algorithms are derived from the discipline of biology, algorithms have been developed inspired by the fields of science such as physics, chemistry, mathematics, psychology and other fields like economics, music, sports etc. (Hussain et al., 2018) (Figure 2.2).

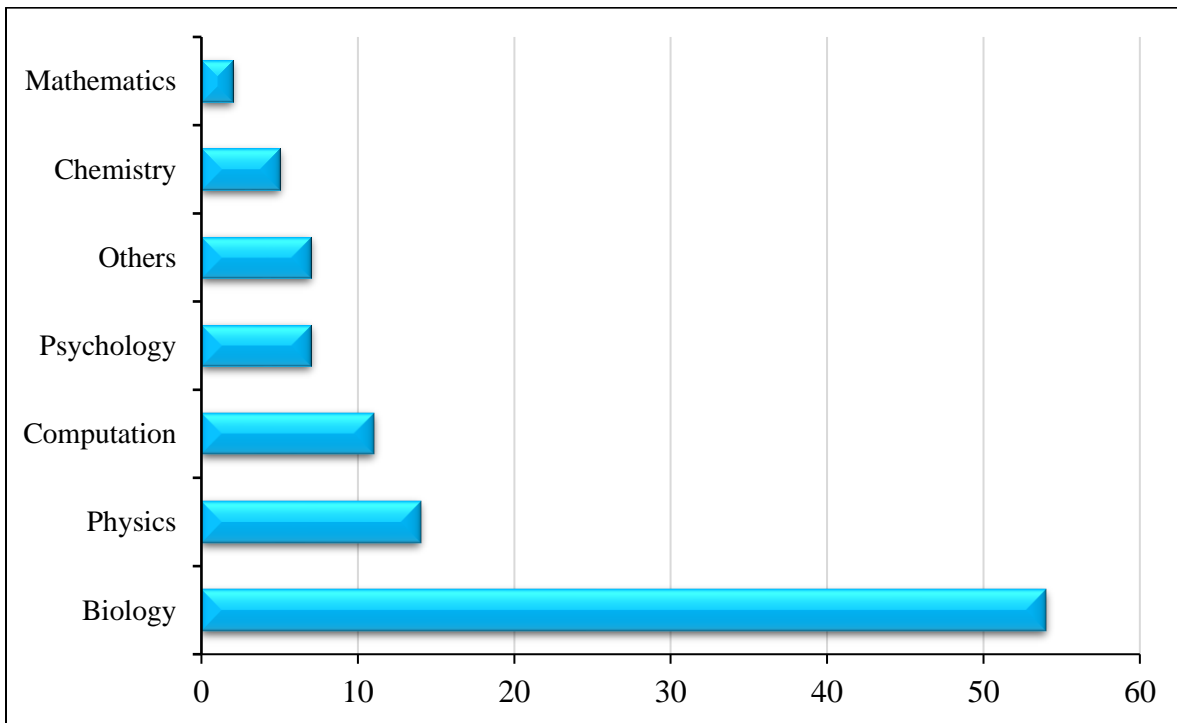


Figure 2.2 Disciplines inspiring metaheuristic algorithms (Hussain et al., 2018)

The success of metaheuristics is attributed to its simple and flexible structure, derivation-free mechanism, and ability to avoid local optima and tune in practice (Memmah et al., 2015). They are inspired by very simple concepts that are easy to understand and adapt to the problem at hand. The metaheuristic algorithms do not require significant changes to the algorithm's structure. This also enables the researchers to modify or hybridize two or more different concepts (Mirjalili et al., 2014). Users are required to know only how to represent their problem to the algorithm (input). They require no gradient information; therefore, they are widely applied to non-analytic, black-box or simulation-based objective functions. Since metaheuristic algorithms are solved stochastically, the algorithms typically start with random initial solutions without any derivative information about the search space. Also, due to the stochasticity of the algorithms, they avoid

local optima and explore the search space extensively. In most cases, complex real-life problems have expensive derivative information and many local optima, so metaheuristic algorithms are a good option to solve them (Bandru and Deb, 2016).

Metaheuristic algorithms have been extensively used to solve problems in various fields like health care (Monga et al., 2021), power systems operations and control (Balaci and Valenzuela, 2004; Varol and Bingul, 2004), renewable energy systems (de Valle et al., 2008), chemical processes (Johnston and Cartwright, 2004), job scheduling problems (Wu et al., 2008), transportation (Teodorovic and DellOrco, 2005), vehicle routing problems (Elshaer and Awad, 2020), telecommunication networks (Ducatelle et al., 2010), batch process scheduling, image processing and pattern recognition problems (Kumar et al., 2021), data mining and analysis (Cheng et al., 2013), and cloud computing (Kalra and Singh, 2015).

The classification of metaheuristics can be done based on inspiration, structure, population, neighborhood, etc. Furthermore, metaheuristics algorithms can be distinguished as nature-inspired or inspired by other sources, population-based vs. single entity solution-based methods, single neighborhood vs. various neighborhood structures, and greedy vs. non-greedy (Behesti and Shamsuddin 2013). This thesis classified the algorithms based on inspiration, focusing on nature-inspired. Nature is a rich source of inspiration, and many researchers have used nature as a reference to derive new methods. Nature-inspired algorithms refer to optimization techniques inspired by one or the other process in nature. Amongst the nature-inspired algorithms, some of the most successful characteristics have been that of the biological system. Therefore, the largest group of nature-inspired algorithms are bio-inspired (Mirjalili et al., 2017; Fister et al., 2013). The physics/chemistry-based and other categories are beyond the scope of this research and will not be discussed here. For further reading on the disciplines used by researchers to develop metaheuristics algorithms and sources of inspiration, readers are referred to Fister et al. (2013), Slowik et al. (2018), and Hussain et al. (2019).

2.3 Bio-inspired Optimization

Bio-inspired metaheuristic algorithms are based on the formation of biological systems, such as genes, evolution process, the social behavior of organisms, foraging, hunting etc. Though bio-inspired metaheuristic techniques may not always yield global optimal results, one can often make a better trade-off between solution quality (optimal solution) and computational time. They have proved to be a suitable, versatile alternative to solve complex, nonlinear practical problems with a broad application base. They are adaptable and provide open-ended, unrestricted problem formulation (no predefined relationship between objective function, decision variables and constraints) (Glover and Sörensen, 2015). These algorithms are further sub-categorized into swarm-intelligence (SI) based and non-SI based algorithms. SI-based algorithms imitate organisms' social/group behavior (like ants, bees, cats, dolphins, fireflies, frogs, glow worms, spiders, wasps, etc.).

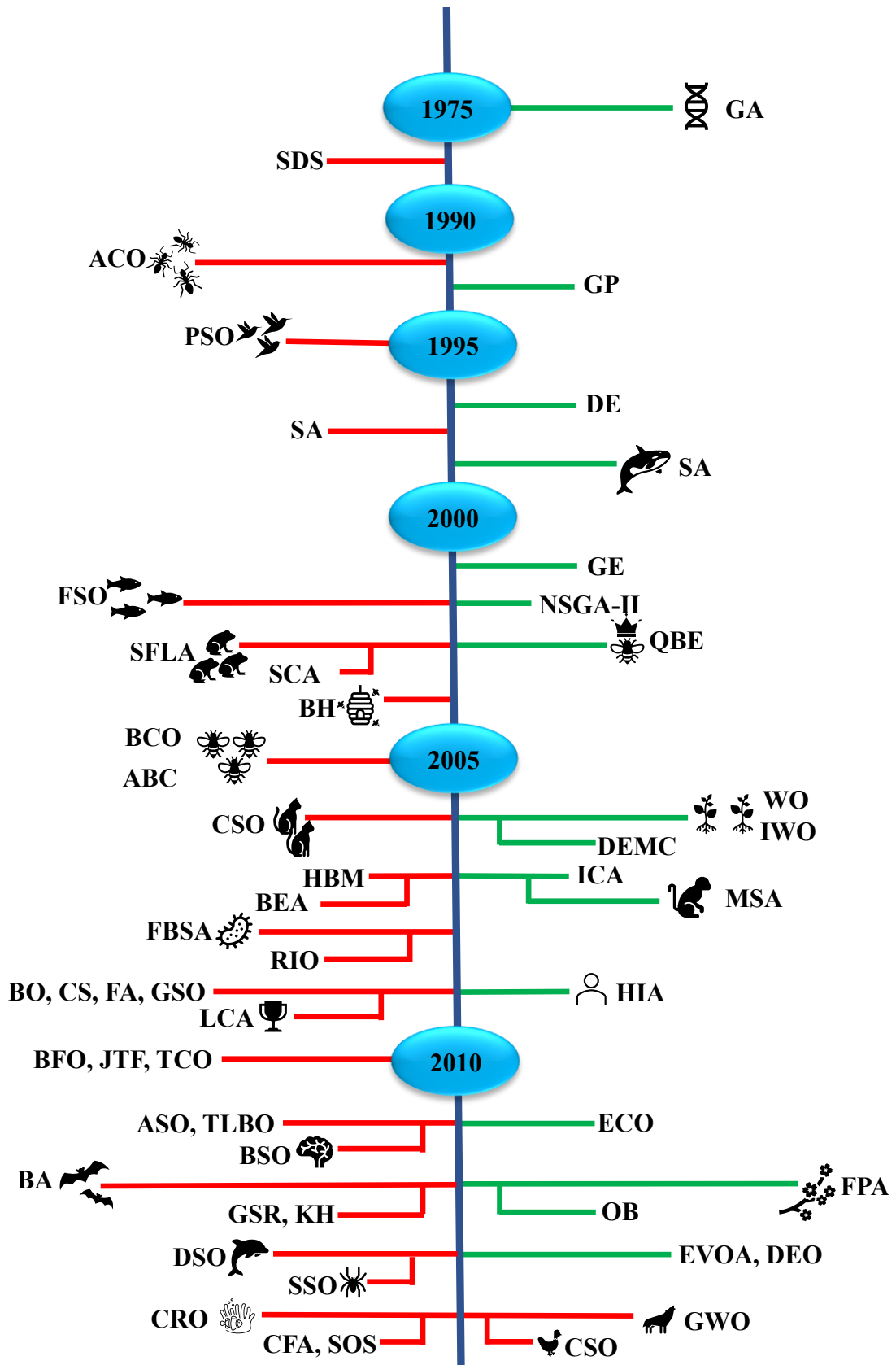
On the other hand, non-SI-based bio-inspired algorithms are based on the properties of organisms other than the swarming behavior (such as pollination of flower, evolutionary strategies, genetics etc.). Other nature-inspired SI-based algorithms (such as Rainfall Optimization Algorithm, Ray Optimization, Gravitational Search Algorithm etc.) have been excluded from this categorization as they are inspired by natural phenomena and not from the discipline of biology. Some of the SI and non-SI-based bio-inspired algorithms are chronologically presented in Figure 2.3. A list with the full name of the algorithms and their reference is provided in Appendix A.

2.3.1 Swarm Intelligence (SI) based algorithms

The term ‘swam intelligence’ was coined by Beni and Wang (1993). SI algorithms are developed based on learnings from the collective behavior of swarms in nature and their complex interaction with no supervision. SI-based algorithms are inspired by social insects’ collective behavior, like ants, termites, bees, wasps, swarms, herd, flock, and shoal of fish, birds or wolves (Olariu and Zomaya, 2005). Many organisms, in nature, live in a community, interacting with each other without centralized decision-making. An organism makes a decision based on its local environment and its interaction with other organisms in the community. The interaction among the organism is believed to be the cause of emergent social intelligence (Yang et al., 2018). SI

approach constitutes an efficient and robust model that simplifies the design of solutions to different problems (Olariu and Zomaya, 2005).

One of the reasons for the popularity of SI-based algorithms is that the information is shared amongst the community members so that the members can accordingly organize, evolve and learn (collective behavior) (Chakraborty and Kar, 2017). The members of a community store the information about the search space over the course of the iterations. SI algorithms usually have fewer parameters to tune (Mirjalili et al., 2014). The self-learning ability and adaptability to environmental variations are significant features that have fascinated researchers and have been recognized in several fields of application for SI algorithms (Fister et al., 2013). Most importantly, SI algorithms are flexible, versatile, and easy to implement, and multiple agents can be parallelized to solve large-scale optimization problems. Many SI-based algorithms are continuously developed, applied, improved and hybridized. Since 2015, more than 21 algorithms have been developed. In the following sections, only some of the most popular, well-established algorithms are described in this thesis.



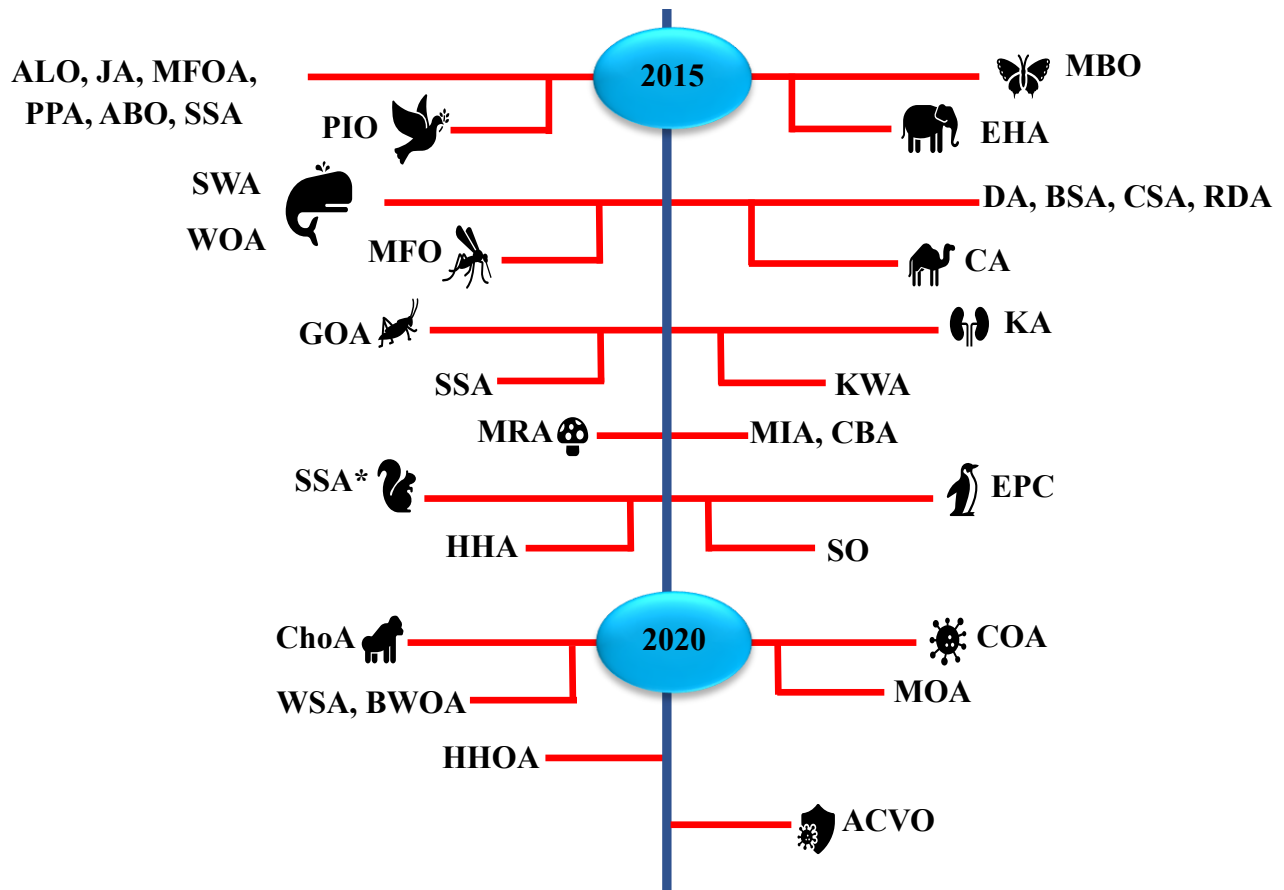


Figure 2.3 Chronology of various bio-inspired optimization techniques developed (red line: SI-based techniques; green line: non-SI-based techniques)

Particle Swarm Optimization (PSO)

Particle Swarm Optimization, developed by Kennedy and Eberhart (1995), is inspired by the movement of a flock of birds or a school of fish to find food sources or shelters. In the algorithm, the particles are initialized with a random solution, and they improve their solution based on the particle's best solution and the global best solution. Each particle is also assigned a velocity vector that contributes to finding the next location of the particle in the search space. Evolution over the iterations occurs due to cooperation between the particles and competition amongst them (Tayfur, 2017). A detailed description of the algorithm is provided in Chapter 3. It is very simple, converges fast and therefore, has gained wide popularity. However, it requires parameter tuning to achieve the global optimal solution. Some of the applications of PSO and its variants in water resources management include reservoir operation (Jahandideh-Tehrani et al., 2020; Chen et al., 2020; Spiliotis et al., 2016), solve optimal cropping and water allocation (Habibi

Davijani et al., 2016), parameter optimization of rainfall-runoff model (Liu, 2009), parameter optimization of water quality model (Afshar et al., 2011), parameter estimation of Muskingum model (Orouji et al., 2012; Moghaddam et al., 2016), non-linear Muskingum model (Chu and Chang, 2009), management of groundwater resources (Gaur et al., 2013), flood control operation (Jahandideh-Tehrani et al., 2020), and land-use allocation (Liu et al., 2014; Ma et al., 2011; Masoomi et al., 2012).

Ant Colony Optimization (ACO)

Ant colony optimization, developed by Dorigo and Caro (1999), is one of the most popular SI-based algorithms based on the foraging behavior of ants using stigmergy. Ants are well-known for their ability to find the shortest paths between their nest and the food source without visual and direct communication. They instead use pheromone deposition on the path to communicate with the other ants. This helps the other ants decide probabilistically to choose the path. They are very flexible animals; when they encounter an obstacle or change in the environment, or if the food source is no longer feasible, they are quick to adapt and scour the space for other food sources. ACO and its variants have been applied in designing water distribution systems (Maier et al., 2003), reservoir operations (Jalali et al., 2005, 2006a and 2006b; Dariane and Moradi, 2008; Guo and Wang, 2010; Yu et al., 2011), derive operating policies for a multi-purpose reservoir (Kumar and Reddy, 2006), parameter estimation in groundwater (Li et al., 2006), optimal control of pumps in water distribution networks (Ibanez et al., 2008), optimal irrigation systems (Nguyen et al., 2017; Tu et al., 2011), and land-use allocation (Liu et al., 2014). A detailed description of the algorithm is provided in Chapter 3. A review of the application of ACO in water resources management can be found in Afshar et al. (2015).

Shuffled Frog Leaping Algorithm (SFLA)

The Shuffled Frog Leaping Algorithm, developed by Eusuff and Lansey (2003), is inspired by a group of frogs searching for food in a swamp. There are many stones next to which the food is usually located in a swamp. Frogs work in groups and share information via memes to quickly locate the maximum food source (Kumar and Yadav, 2022). There are three main stages adopted in the algorithm: portioning, local search and shuffling. In the algorithm, the frogs in the swamp are portioned into small groups called memplexes to perform a local search. They are ranked from

best to worst fitness level based on their location. A frog can be influenced by the other frogs and evolve through memetic evolution within the memplex – the worst frogs are directed to leap towards the location of the best frog. Then the memplexes are shuffled, thus increasing the probability that all frogs move towards the best solution. The advantages of using SFLA are that it combines the benefits of the memetic algorithm, PSO-based local search, and shares information parallelly during local search (Du and Swamy, 2016). Many variants of SFLA have been developed over the years, as described by Sarkheyli et al. (2015) and Maarroof et al. (2022). SFLA has been applied to designing water distribution networks (Eusuff and Lansey, 2003), groundwater modelling and water distribution systems (Eusuff et al., 2006), large-scale water supply systems (Chung, 2009), to solve optimal reservoir operation (Li et al., 2018; Sun et al., 2016; Yang et al., 2019), and optimal allocation of water resources (Fang et al., 2018).

Artificial Bee Colony (ABC)

Artificial Bee Colony, developed by Karaboga (2005), is based on honeybee swarms' foraging behavior. In a bee colony, bees leave the hive in search of a food source (nectar). After finding nectar, the bees store it temporarily in their stomach. Upon returning to the hive, they unload the nectar into the hive and perform a waggle dance indicating the location and nectar quantity at the food source. This is a way to recruit new bees to explore the richest food sources. Four types of bees are identified in a colony – employed bees, unemployed bees, scout bees, and onlooker bees. In the algorithm, the food sources represent the probable solution, the number of employees bees is the same as the number of probable solutions, and the quality of nectar from a food source is used to evaluate the fitness of a bee (Schiezaro and Pedrini, 2013). It is the job of employed bees to search for the food source and then inform the location and quality of the onlooker bees. The better the quality of the food source, the higher the number of times the information is shared, thus increasing the probability of recruiting onlooker bees to choose the food source. Once an onlooker bee picks a food source to explore, it becomes an employed bee. And when an employed bee exhausts search for a better quality of food but can't find it anymore, the food source is abandoned, and the bee becomes a scout bee and searches for a new food source randomly. This process is repeated until an optimal food source is found.

ABC is flexible, simple, robust, easy to implement and capable of performing a local and global search. However, the sequential processing of ABC is slow, and tuning parameters such as

scout, onlooker and employed bees are required to use the algorithm (Li and Feng, 2020). Some of the well-known variants of bee colony include Bee Colony Optimization proposed by Teodorovic and Dell'Orco (2005), Bee Algorithm proposed by Pham et al. (2007), Bee Swarm Optimization by Akbari et al. (2010), Weighted Bee Colony Optimization by Moayedikia et al. (2015), and improved Artificial bee colony (iABC) by Mann and Singh (2019). ABC and its variants have been applied in the fields of groundwater management (Boddula and E, 2018), groundwater prediction (Li et al., 2019), reservoir optimization (Ahmad et al., 2016; Moeini and Soghrati, 2020), and designing water distribution networks (Li and Feng 2020).

Cuckoo Search (CS)

Cuckoo search is based on the specific egg-laying (parasitism) and breeding of some cuckoo species. It is developed by Yang and Deb (2009). Cuckoo birds lay their eggs in some other birds' nests, and as long as these are not recognized by the host bird as a foreign substance and destroyed or abandoned, they grow up to become cuckoo birds. Therefore, cuckoo birds must find the best environmental features and groups that allow the best breeding (Rajabioun, 2011). To simplify the search, in the CS algorithm, three conditions are assumed: 1) a cuckoo bird lays only one egg at a time in a random nest (solution), 2) the nest containing the best egg is the best nest, and only the best nest is accepted to the next generation, and 3) discovering of the cuckoo eggs by the host bird is dependent on probability; if discovered, the host bird either deserts the nest or destroys the egg. Also, the number of host nests is initialized at the beginning of the algorithm. This ensures that each bird has only one solution and better solutions are carried over to the next generations, thus, guiding all the birds towards the optimal solution (Yang and Deb, 2014). The formulation can be modified for a complex problem to allow several eggs to be laid in a nest. The fitness of a solution is proportional to the value of the objective function of the solution (Yang, 2014).

CS uses a combination of random local walk and global exploration. The random walk is similar to the Markov Chain, where the next position depends on the current position and the transition probability. An entry-wise product of Lévy flight is also used, which utilizes Lévy distribution to select random step lengths. The most significant advantage of CS is the use of Lévy flight for global search. This yields infinite mean and variance, thus, enabling CS to explore the search space more efficiently than other standard processes. The local search of CS is very

intensive, and search space is explored more efficiently on the global scale; consequently, the global optimal solution is found with a higher probability (Yang and Deb, 2014). Rajabioun (2011) developed a variant of CS, the Cuckoo Optimization Algorithm. It performs a continuous awareness search based on a cuckoo bird. CS has been applied in multiple fields of water resources management, including calibration of a groundwater flow model (Valeto et al., 2019), reservoir operation (Boindala and Arunachalam, 2019; Yasar, 2016), design of water distribution networks (Pankaj et al., 2020), water productivity (Upadhyaya and Upadhyaya, 2021) and crop planning (Mohammadrezapour et al., 2017; Rath et al., 2019) etc. Detailed information on CS, its development, and recent applications can be found in the review articles by Joshi et al. (2017) and Guerrero-Luis et al. (2021).

Firefly Algorithm (FA)

The firefly algorithm, developed by Yang (2009), is based on the flashing behavior of swarming tropical fireflies in nature. The flashing behavior fulfills two fundamental functions — attract prey and mating partners; protect the firefly from predators. FA is a simple, flexible, easy-to-implement algorithm (Slowik et al., 2018). It finds the optimal solution using greedy search with randomness introduced into the search function. FA works with three assumptions: 1) all fireflies are unisex (attraction irrespective of the sex of a firefly), 2) the attractiveness of a firefly is proportional to its brightness, and it decreases with increased distance, and 3) the objective function determines the brightness of a firefly. Decentralized decision-making and self-organizing behavior are two key characteristics of the firefly algorithm. The flies' social life is dedicated to the reproduction of fireflies and foraging, which depends on the fireflies' flashing. However, it doesn't mean they are autonomous; the collective decision is related to the fireflies' flashing pattern, which is the most important biological function used in the firefly algorithm (Verma, 2020).

In this algorithm, the brightness of the flash is used to evaluate the fitness of a firefly. The fireflies are initialized with random solutions, and the fitness is evaluated. A firefly with low fitness tries to improve by moving towards the fittest firefly. The best firefly at the end of the algorithm would be the optimal solution. It is capable of finding both global and local solutions synchronically and effectively. It is especially convenient for parallel implementation as fireflies work independently (Kumar and Yadav, 2022). FA has many parameters that require fine-tuning,

including the maximum number of iterations, number of fireflies, random parameters based on a distribution, absorption coefficient, attractiveness parameter, and scaling factor (Wang et al. 2018). Many variants of FA have been developed over the years to increase the algorithm's applicability in terms of modification or hybridization. A detailed account can be found in Verma (2020). In water resources management, FA has been applied to estimate water demand (Wang et al., 2017a, Wang et al., 2018), water allocation (Wang et al., 2017b), water distribution system (Tahershamsi et al., 2014), evaporation prediction (Moazenzadeh et al., 2018), optimal reservoir management (Garousi-Nejad et al., 2016; Kangrang et al. 2019), and groundwater management (Kazemzadeh-Parsi et al., 2015) amongst others.

Bacterial Foraging Optimization (BFO)

Bacterial Foraging Optimization, developed by Passino et al. (2010), is based on the foraging of the bacteria using chemotaxis. Bacteria undergo chemotaxis to move towards a landscape of nutrients and avoid environmental toxins. When the bacteria encounter a food source that is sufficient, it reproduces itself by binary fission. If it encounters an attack or change in the environment, it gets destroyed, or a group gets dispersed into a different place. In the algorithm, each bacterium moves towards global optimum using tumble or swim in the chemotaxis. When a bacterium swims, it changes the location but moves in the same direction, whereas when it tumbles, it chooses a random direction. Each bacterium signals other bacteria to swarm together upon finding a food source. Since this process may be stuck at local optima, some bacteria (low fitness) are dispersed or killed after a threshold number of reproductions by the fittest bacteria. The dispersion and elimination are dependent on the user-defined probability of elimination parameter. This keeps the swarm size constant and ensures only the fit bacteria move forward in the iteration towards nutrient-rich food sources. Many variants of BFO have been developed and discussed in detail by Das et al. (2009). In water resources, it has been applied to detect groundwater possibility (Kapoor et al., 2012), predict water resource demand (Zhang et al., 2019), and solve conjunctive use of surface and groundwater resources (Sampathkumar et al., 2021).

Bat Algorithm (BA)

The bat algorithm, developed by Yang and Gandomi (2012), is based on the foraging by the microbats using echolocation. They emit a loud pulse and hear the echo that bounces back from their prey, obstacles, and roosting crevices. In the algorithm, three assumptions have been made: 1) all bats use echolocation to locate the distance, and they are aware of the difference between prey, obstacles and background barrier, 2) bats search for prey with a random velocity, fixed frequency, varying wavelength, and loudness, and they adjust the wavelength and rate of pulse emission depending on the prey proximity, 3) range of variation in loudness is provided. The bats are initialized with pulse rates and loudness; pulse frequency for every location is also defined. Each location is a candidate solution, and the objective is to find the best location. The bats move to new locations by adjusting the frequency and calculating the velocity of the subsequent position based on the current velocity and location. The algorithm uses a local random walk to increase the ability of the bats to search.

BA is easy to implement and flexible. It has fast convergence and yields the best solution in less time. However, it requires parameter tuning as convergence depends on wavelength and emission coefficient (Gandomi et al., 2013). The convergence is affected if the proper tuning parameters, such as wavelength and emission coefficient, are not done. Yang and He (2013) discuss its application in various fields. BA has been used in reservoir operation (Bozorgg-Haddad et al., 2014; Ethteram et al., 2018a; Zarei et al., 2019), rainfall forecast (Kuok et al., 2019), suspended sediment predictions in a river (Banadkooki et al., 2019), and improving Muskingum flood routing (Ethteram et al., 2018b).

Grey Wolf Optimizer (GWO)

The Grey wolf optimizer, developed by Mirjalili et al. (2014), is based on the hunting and social hierarchy of the grey wolves. The wolves are divided into four classes – alpha (leader of the pack), beta (subordinate to alpha and assists in decision-making), delta (subordinate to alpha and beta), and omega (submits to the other three classes of wolves). While hunting, grey wolves circle their prey, and the hunting is guided by the alpha wolf and assisted by beta and delta wolves. In the algorithm, the first three best solutions are assigned the alpha, beta and delta positions and the rest of the solutions are assumed to be omega. The omega solutions are updated based on the alpha,

beta and delta locations in the search space. Vector coefficients are introduced in the algorithm to ensure divergence of the pack to find better solutions and introduce random behavior. Thus, avoiding local optima and ensuring exploration of the search space. Hybridization of GWO with other well-established algorithms has been developed by Wang and Li (2019). In water resources management, GWO has been applied to water quality assessment and classification (Sweidan et al., 2015), optimization of irrigation water distribution (Choopan and Emami, 2019; Shahverdi and Maestre, 2022), and prediction of water storage in a dam (Emami et al., 2020).

Other popular SI-based algorithms include Fish Swarm Optimization (Li et al., 2002), Cat Swarm (Chu et al., 2006), Bumblebees Optimization (Comellas and Matrinez, 2009), Krill Herd (Gandomi and Alavi, 2012), Social Spider Optimization (Cuevas et al., 2013), Teaching Learning Based Optimization (Rao et al., 2011), Moth-flame optimization algorithm (Mirjalili, 2015a) and Whale Optimization Algorithm (Mirjalili and Lewis, 2016).

2.3.2 Non-SI-based algorithms

Amongst the non-SI-based algorithms, the most prevalent are the evolutionary algorithms (EA). They are inspired by the ‘neo-Darwinian paradigm for simulating the natural evolution of biological systems’ (Du and Swamy, 2016). Though these algorithms were developed in the 1960s, they remained un-investigated until the mid-1980s (Coello Coello, 2001). These algorithms have three basic operators named crossover, mutation, and selection. Evolutionary algorithms are further classified into genetic algorithms, genetic programming, evolution strategies, evolution programming, and differential evolution. Only a brief explanation of these classifications is provided in this section.

Evolutionary Strategies (ES)

Evolutionary Strategies, introduced by Schwefel, Rechenberg and Bienert in the 1960s, are inspired by mutation and recombination processes similar to GA (Rudolph, 2012). The key difference between the two algorithms is the self-adaptive mutation rates. While GA explores the search space by recombining the solutions and preserves a genetic link, ES works on an individual solution and its offspring level. Its selection process is deterministic (Ab Wahab et al., 2015). There are three different types of adaptive mutation processes available. a) (1+1)-ES – only one offspring is produced by a parent; if the offspring performs better than the parent, it becomes a

parent in the next generation; otherwise, it is eliminated; b) $(1+\lambda)$ -ES produces λ offsprings, only the best out of λ offsprings can become a parent in the next generation, everything else is eliminated; c) $(\mu/\rho +, \lambda)$ -ES is often used as standard ES process where λ offsprings are produced by ρ parents. If '+' is selected, the parent generation competes with the offsprings; if ',' is selected, they are eliminated, and only offsprings compete amongst themselves to be selected for the next generation (Hansen et al., 2015). Different adaptation strategies to yield better performance have resulted in the development of multiple variants of ES.

Evolutionary Programming (EP)

Fogel proposed the idea of evolutionary programming in the 1960s (Fogel, 2012). EP's initialization, mutation, and evaluation processes are the same as GA. The difference between EP and GA is that EP does not undergo the crossover process to create offspring. The selection process in EP is stochastic. A chromosome competes against a user-defined number of other chromosomes, and the weak chromosomes are eliminated. EP is apt to solve problems with many local optimal solutions (Lee and El-Sharkawi, 2008). The concepts of ES and EP were used to develop Genetic Algorithms.

Genetic algorithm (GA)

Developed by Holland (1975), the Genetic Algorithm is one of the most famous EAs. It is based on the Darwinian principle of natural selection, a process of genetic evolution. A chromosome is filled with genes. Parent chromosomes create the offsprings through the crossover operation (mix and match of genes). If the offspring chromosome is strong, it has better adaptability, will survive and be selected to pass on the genes to the next generation. Chromosomes that aren't suitable are removed. In the algorithm, the problem parameters are regarded as the genes of a chromosome. A fitness value (highly related and proportional to the objective function) is used to reflect a strong chromosome. Three genetic operators- selection, crossover, and mutation, are used to improve the current solutions chosen from the initial generation and select the best offspring to carry over to the next generations. This is repeated until the stopping criteria is met. One of the notable improvements/ modifications of GA is the Non-dominated Sorting Genetic Algorithm II (NSGA II, Deb et al., 2002). Variants of GA has been successfully applied to solve groundwater monitoring and management (McKinney and Lin, 1994; Kollat and Reed, 2006),

irrigation water management (Chen, 1997), designing water distribution network or pipelines (Goldberg and Kuo, 1987; Haghghi and Bakhshipour, 2012), reservoir management (Sharif and Wardlaw, 2000; Reddy and Kumar, 2006; Kim et al., 2008), selection of agricultural BMPs (Liu et al., 2013b), water management (Gino Sophia et al., 2020) in water resources management. A review of the application of GA and its variants in water resources management is provided by Nicklow et al. (2010) and Rani et al. (2013).

Genetic Programming (GP)

David Goldberg coined the term Genetic Programming, and the algorithm was developed by Koza (1992) and is similar to the workings of GA. The difference between the two is the solution and selection operation representation. The term chromosome represents a solution to the problem in GA, whereas in GP, it represents a solution program. To reproduce, GA selects the user-defined percentage of robust candidate solutions (based on fitness). In contrast, in GP, the selection is based on the probability given to each program of GP is dependent on the program's fitness level and based on the objective function one or more programs are selected (Ab Wahab et al., 2015). GP is often used to solve problems where the variables of the problem are not fixed values. The application of GP in water resource management was kick-started by developing the weights matrix for ANN to study the rainfall-runoff (Savic et al., 1999). It has since been applied in parameter optimization of models (Pelletier et al., 2006), to optimize ANN modelling of the rainfall-runoff process (Nourani et al., 2011), pan evaporation modelling (Güven and Kisi, 2013), designing low-impact urban development (Zhang et al., 2013), reservoir operation (Akbari-Alashti et al., 2015), flow routing (Fallah-Mehdipour et al., 2016), groundwater monitoring (Prakash and Datta, 2014; Cobaner et al., 2016), prediction of monthly streamflow (Ravansalar et al., 2017), and runoff modelling (Heřmanovský et al., 2017). Mehr et al. (2018) and Mohammad-Azari et al. (2020) provide a detailed review of the application of GP in water resources management.

Differential Evolution (DE)

Differential Evolution, developed by Storn and Price (1997), is inspired by the self-organization of the simplex search algorithm (Nelder and Mead, 1965) and reproduction strategy. Every generation in DE is created based on the classical EA operators to evolve a randomly generated initial population to a final solution. The mutation is the first operation performed by

DE, followed by crossover to increase the diversity of the population. Selection of the best offspring is the next operation until the stopping criteria is reached. Many modifications and hybridization of DE have been developed over the years, including Differential Evolution Markov Chain (DEMC by Braak, 2006). The Swedish Meteorological and Hydrological Institute adopted DEMC as an auto-calibration method in their hydrological model. However, the first application of DE in water resources management was on reservoir operation by Reddy and Kumar (2006). Other applications include but are not limited to the water distribution network (Vasan and Simonovic, 2010; Zheng et al., 2012; Moosavian and Lence, 2017), irrigation planning (Raju et al., 2012), optimal cropping pattern (Otieno and Adeyemo, 2010), reservoir optimization (Ahmadianfar et al., 2017; Nwankwor et al., 2013; Regulwar et al., 2010), coastal subsurface water management (Karterakis et al., 2007), and groundwater management (Gurarslan and Karahan, 2015).

The application of some more non-SI-based algorithms like Dolphin Echolocation Optimization and Invasive Weed Optimization is being evaluated by researchers but is not covered in this thesis. It can be seen from the extensive review of the literature presented in the aforementioned sections that bio-inspired optimization techniques are highly versatile. They can solve complex problems by using the emergent intelligent behavior of the population. This is a very critical functional aspect of bio-inspired optimization that can be applied to various problems at different stages of IRBM.

2.4 Agent-based model (ABM)

Apart from system component optimization, it is critical to understand the human aspects/influence on the system components. Rather than defining the problem as a global function, the results would depend on the community's actions and interactions. In this regard, the agent-based model serves as a tool through which optimized management policies that suit the river basins can be developed with contributions from the stakeholders of the basin. ABM is a powerful simulation technique that explores agents' behavior in a real-life system. ABM has three main components – agents (autonomous with behavioral rules), the environment (that enables action) and their interaction. ABM simulates the emergent behavior of the agents based on the user-defined behavioral rules and their interaction with the environment. It provides micro-level assessments considering the specific river basin constraints, capacities and stakeholders' behavior.

With ABM, behavioral aspects of the stakeholders can be incorporated to find optimal policies from a planning and policy development perspective. A framework developed with ABM can capture individual interaction and response from society with respect to the policy or infrastructural changes suggested by the decision-making body. It has been applied to model the behavior of water users and managers on a catchment scale (Huber et al., 2021), adoption of water-saving methods (Galán et al., 2009), simulate and the effect of water use and land use on regional groundwater (Reeves and Zellner, 2010), adoption of green infrastructure (Montalto et al., 2013) to name a few. A detailed review of the application of ABM in environmental applications like rural water management, flood mitigation, and agricultural land use can be found in the review articles by Hare and Deadman (2004) and, recently, by Berglund (2015).

To summarise, the field of bio-inspired algorithms is an emerging branch of computational optimization. It is based on the concept and inspiration of the evolution of biological creatures in nature. Though bio-inspired algorithms have been well established for the last few decades, it is still an evolving field with new robust and competing techniques and hybridization of the existing algorithms being developed and tested day-by-day (Kar, 2016). Their high performance has received particular attention over the past few years. They can solve real-world high-dimensional complex problems resourcefully and with high accuracy and therefore find the wide application (Selvaraj et al., 2015). This thesis explores the application of bio-inspired algorithms with respect to IRBM.

3. Spatial distribution of mitigation measures to reduce total nitrogen concentration using Ant Colony Optimization and Particle Swarm Optimization

Abstract

In this study, an attempt has been made to explore the effectiveness of metaheuristic bio-inspired algorithms in performing discrete combinatorial optimization. The study aims to spatially distribute mitigation measures to reduce long-term annual mean TN concentration at the river basin's outlet. Two well-known and established bio-inspired algorithms, Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO) are used to distribute the measures within the basin. A case study of the Fuhse river basin simulated in HYPE is used. Nine different measures under four categories are provided to the algorithms to distribute at crop and subbasin levels to address point and non-point source pollution. The measures include reducing fertilizer and manure application, reducing tillage and increasing the efficiency of wastewater treatment plants. The results show that both algorithms have successfully distributed the measures within the basin to reduce long-term annual mean TN concentration. Their performance is on par with each other and achieved an annual mean reduction of 0.9 mg/l (18.26 %) over six years. With this study, we prove the strength and flexibility of bio-inspired algorithms to be applied in the spatial distribution of measures addressing river basin management.

Keywords: ant colony optimization, particle swarm optimization, total nitrogen management, spatial distribution, mitigation measures.

Highlights:

- Two popular, well-established bio-inspired algorithms were tested for a single objective combinatorial discrete optimization problem in IWRM;
- The objective of the study was to maximize long-term total nitrogen reduction at the basin outlet by spatially distributing mitigation measures within the river basin;
- Ant colony optimization and Particle swarm optimization can successfully address spatial distribution problems in a river basin.

3.1 Introduction

According to European Environment Agency, the two primary sources of total nitrogen (TN) are anthropogenic diffused and point sources. In the anthropogenic diffused sources, 50-80% of the total nitrogen load is attributed to agricultural activities, while municipal wastewater constitutes 75% of the point source discharges (European Environment Agency, 2005). The adverse impacts of nitrogen on the ecosystem and human health are well known and are discussed in detail by de Vries (2021). To abate the pollution caused by nitrogen at the catchment scale, the Water Framework Directive (WFD, Directive, 2000/60/EC) and the Nitrates Directive (Council Directive 91/676/EEC) have issued mitigation measures or best management practices. Fassio et al. (2005) used a GIS environment on agricultural land to investigate the impact of alternative policy measures developed at a European scale to reduce nitrogen pressure from European agricultural lands. Their study adopted the European Environmental Agency's DPSIR approach (Driving force, Pressure, State, Impact, Response) of a multi-criteria decision support system to evaluate possible alternative solutions for policy implementation. Volk et al. (2009) modeled the upper Ems River basin in Germany using SWAT and assessed the impacts of eight consecutive land use and management scenarios. They concluded that regional landscape and land use distinctions are required to reach the target TN concentration limit for the basin.

Laurent and Ruelland (2011) modeled the Oudon river basin in France to assess the impact of seven alternative best management practices (BMPs) on nitrogen flow through the basin. Reduced fertilization showed a maximum reduction of nitrate flow, followed by no-tillage, conversion to catch crops, and the use of filter strips. They concluded that modeling at different catchment scales aids in analyzing the impacts of the practices. However, a combination of BMPs is required to improve water quality drastically. Panagopoulos et al. (2011) also reached a similar conclusion from their study on the Arachtos basin in Greece using SWAT. They analyzed the establishment of filter strips and reduction of fertilization combined with contour framing and no-tillage as BMPs to reduce sediment, nitrate-nitrogen, and total phosphorus input to surface waters. They inferred that only combined measures in small catchments could considerably reduce several pollutants. The long-term impact of point and non-point sources of pollution and the effectiveness of BMPs to improve water quality were analyzed for the Kielstau catchment in Germany by Lam et al. (2011). Their results indicated that up to 20 % reduction in average annual load of nitrate and total

nitrogen was achieved by implementing one BMP at a time, and up to 53.9% reduction of nitrate was achieved by the combination of BMPs. According to Merriman et al. (2019), implementing multiple BMPs in combination (like filter strips and grassed waterways) significantly reduced sediment and nutrient loads compared to a single BMP implementation.

The efficacy of the combinations of measures to achieve the target limits depends on their spatial distribution in the river basin. However, this can be tricky as the river basin is a complex entity where the hydrological process is affected by the number of sub-basins, multiple land-use characteristics, pollutant sources, hydro morphological modifications, farming practices, and climate in each sub-basin, to name a few. Dietrich and Funke (2009) discussed integrating catchment models into a long-term iterative strategic planning and decision-making process. They analyzed four strategic scenarios for the spatial distribution of measures to reduce total phosphorus from point and non-point sources in the Werra River basin in Germany.

Panagopoulos et al. (2013) used a decision support tool with multi-objective optimization using an elitist Genetic Algorithm (Deb et al., 2002) to identify the distribution of low-cost BMPs in a basin to ensure good water quality. They used a BMP database containing the sum of annual total phosphorus (TP) concentration, $\text{NO}_3\text{-N}$ losses and cost of implementation. Their study yielded one hundred optimal solutions, which were then simulated in SWAT to evaluate the TP and $\text{NO}_3\text{-N}$ concentration in the river. Policymakers, stakeholders, and resource managers need mechanisms to assess which combination of measures can be adopted to achieve the target limits for their basin (reducing the total nitrogen). In this regard, metaheuristic algorithms constitute an extensive collection of optimization techniques inspired by concepts of natural phenomena. They are increasingly used to solve challenging tasks like model calibration, planning, design and operation of water resources systems due to the versatility and adaptability of the algorithms (Maier et al., 2019). Their ability to solve complex, non-linear problems with a significant degree of complexity is advantageous to solve the optimal spatial distribution of measures in a river basin. Amongst the metaheuristic algorithms, swarm intelligence-based algorithms are popular among researchers as they are robust, flexible, and scalable to complex problems (Oliveira et al., 2020). This paper considers two well-established algorithms: Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO).

Dorigo and Caro (1999) developed the metaheuristic ACO technique from their multiple works on ant systems. The first application of ACO in water resources was by Abbaspour et al. (2001) to estimate the hydraulic parameters of unsaturated soils. From then on, ACO has been widely applied to numerous water resources management problems like reservoir operation and scheduling (Jalali et al., 2006; Kumar and Reddy, 2006), design of water distribution networks (Maier et al., 2003; Zecchin et al., 2007), stormwater and sewer systems (Afshar, 2010), environmental flow management (Szemis et al., 2012; 2014) etc. Madadgar and Afshar (2008) developed an improved continuous ACO for specific water resources requiring continuous domains or decision spaces. Their algorithm robustly identified the optimal solution for a single hydropower reservoir operation problem. Liu et al. (2012) used Multiple-type Ant Colony Optimization for optimal Multiple Land Allocations (MACO-MLA) to a large-scale catchment in China to optimize the land-use allocation with conflicting objectives. They compared it with the Genetic Algorithm (GA, Holland, 1975) and Simulated Annealing (SA, Kirkpatrick et al., 1983). They concluded that MACO-MLA generates better utility values than SA and GA.

Skardi et al. (2013) used ACO to evaluate wet ponds' efficient sizing and location for a minimum cost to reduce sediment yield. They simulated a hypothetical basin in SWAT. They determined that ACO performed well and yielded the best location and size of the ponds for minimum cost to reduce sediment yield at the outlet of the wet ponds. Nguyen et al. (2016) applied a combination of static and dynamic decision variable options with ACO to optimize crop and water allocation. The authors used a graph structure to represent the decision space. Their study concluded that the ACO with dynamic decision variable options consistently performed better and was computationally efficient than static decision variable options and linear programming. Ostfeld (2011) reviewed the application of ACO for water resources system analysis and the challenges faced by researchers. A more recent review of ACO in water resources management is discussed by Afshar et al. (2015).

The reliability and robustness of ACO has been well established in solving benchmark problems of water distribution networks (Maier et al., 2003; López-Ibáñez et al., 2008; Zecchin et al., 2003). Analogy can be drawn from the water distribution network problem (nodes, pipe sizes and connections) to the current study (mitigation measures) as it also involves discrete

combinatorial optimization. Therefore, in the attempt to apply bio-inspired algorithms for IRBM aspects, ACO has been chosen to be used in this study.

PSO, proposed by Kennedy and Eberhart (1995), is a stochastic optimization technique based on the swarm's cooperation to find the optimal solution. Due to its easy-to-implement and straightforward structure and fast convergence, PSO has gained popularity to solve complex real-world problems. PSO and its variants have been applied to various problems in water resources management, like training an artificial neural network to predict real-time water levels in a river (Chau, 2004) and reservoir operation (Baltar and Fontane, 2008; Fallah-Mehdipour et al., 2011; Ostadrahimi et al., 2012; SaberChenari et al., 2016), parameter optimization of hydrological model (Zakermoshfegh et al., 2008), stormwater network design (Afshar, 2010), land-use spatial optimization (Ma et al., 2011), design and optimization of water distribution networks (Ezzeldin et al., 2014; Surco et al., 2018), and modeling and predicting water quality parameters (Aghel et al., 2019). Liu et al. (2012) used multi-objective PSO to solve the land use zoning problem at a county level. They concluded that integrating the GIS information with multi-objective PSO is a promising and efficient approach to solve the land use zoning problem. Liu et al. (2013a) used hybrid PSO and system dynamics to solve urban land use allocation at a macro-level, considering the socio-economic variables. They concluded that their combined model reproduces the complex land use behavior at multiple scales and develops alternative land-use patterns based on user-generated scenarios. A comprehensive overview of PSO and its variants is discussed by Zhang et al. (2015), Wang et al. (2018), and Jain et al. (2018). Jahandideh-Tehrani et al. (2020) discussed the application of PSO in water management. Due to a wide range of applications in water resources problems, including spatial optimization of land use, PSO and ACO are selected to be evaluated in this study. PSO is a versatile and flexible algorithm with simple straightforward equations and fast convergence. Due to its ease of implementation and it being a swarm intelligence-based optimization algorithm similar to ACO, it has been used in this study to compare or contrast the results of ACO.

This study explores the effectiveness of metaheuristic bio-inspired algorithms in performing a discrete combinatorial optimization of the spatial distribution of mitigation measures to reduce long-term TN concentration at the river basin's outlet. We adopt an approach where the simulation results of the selection of measures by the algorithms are not pre-determined but instead unfold

during the iteration process based on the hydrological model computation, which to our knowledge, has been attempted for the first time. This enables the algorithms to be used on other catchments with minimal code revision. Section 3.2 describes the study area, measures to be distributed, implementation level in the search space and a brief description and adaptation of ACO and PSO to distribute the measures spatially. The results are presented and discussed in Section 3.3, while conclusions and recommendations are given in Section 3.4.

3.2 Materials and Methods

3.2.1 Study Area

In this study, the upper part of the Fuhse River basin in Lower Saxony, Germany, with a catchment area of 385 km² is simulated (Figure 3.1).

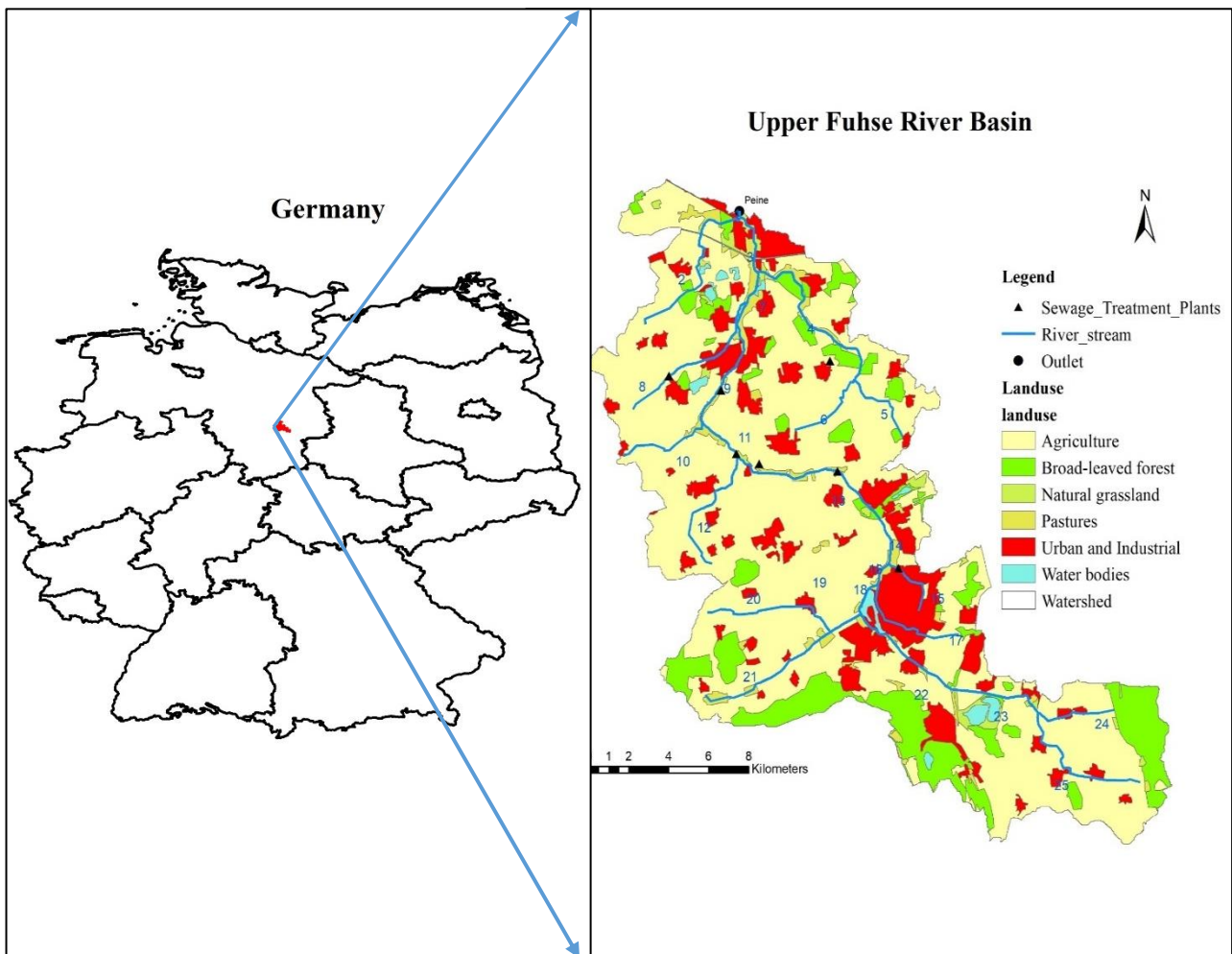


Figure 3.1 Upper Fuhse river basin, Germany

According to the Bundesanstalt für Gewässerkunde (BfG – German Federal Institute of Hydrology), the ecological and chemical status of the Fuhse River as of December 2015 is categorized as ‘bad.’ The deterioration of the river is attributed to diffused pollution from agricultural activities, the discharge from the wastewater treatment plants in the basin, the mixing of rainwater runoff and sewage, and heavy hydro morphological modifications of the river. Therefore, the upper Fuhse river basin is an apt location for a case study to analyze the spatial distribution of measures to reduce total nitrogen (TN) concentration in the river.

The basin is simulated in the Hydrological Predictions for the Environment model (HYPE, <https://www.smhi.se/en/research/research-departments/hydrology/hype-our-hydrological-model-1.7994>). HYPE is a dynamic, semi-distributed, and process-based hydrological and nutrient transport model developed by the Swedish Meteorological and Hydrological Institute (Lindström et al., 2010). The climate in the study area is influenced by the oceanic conditions of the North Sea. The average annual precipitation of 718 mm and 645 mm was recorded in stations Salzgitter-Lichtenberg and Lengede, respectively, between 2000 and 2016, with July and August being the wettest months of the year. The climate data for the study area was collected from the German weather service (Deutscher Wetterdienst). Data from 26 rainfall stations within a 25 km radius around the basin was used to derive interpolated rainfall for the subbasins using the Inverse Distance Weighting method (IDW). And for temperature, solar radiation, relative humidity and wind speed, data from stations within a 30 km radius was interpolated using the IDW method.

The national medium-scale soil map and database, BÜK 200, describes the varieties of soils in the catchment. The various soil types identified within the basin are podosol (arenic), regosol, luvisol, pseudogley (stagnosols), moor soil, gley and black soil. The most prominent soil type in the basin is podosol and black soil. The major land-use types, according to the 2006 CORINE landcover map, are agriculture (67.2%), urban settlements (14.2%), and forest (13%). There are also some pastures (3.4%), natural grassland (1.1%) and water bodies (1.1%) in the basin. Statistical agrarian information published by the Agricultural Chamber of Lower Saxony (Landwirtschaftskammer Niedersachsen) is used to estimate the crop distribution in the basin. Major crops grown in the basin include winter wheat, winter barley, sugarbeet, summer barley, rapeseeds, potatoes and corn silage. Data on streamflow, water quality and discharge from

wastewater/sewage treatment plants (STP) were provided by the Lower Saxony Water Management, Coastal Defense and Nature Conservation Agency (NLWKN).

The Fuhse river shows pollution by nutrients, mainly attributed to inflow from wastewater treatment plants (point sources) and agricultural activities (non-point sources). This study considers seven wastewater treatment plants that discharge their treated wastewater into the Fuhse River network. Since no data on the amount of fertilizer applied and the application time were available, recommendations of the Agricultural Chamber of Lower Saxony are used in the model, assuming non-point nutrient inputs from “good agricultural practice.”

A global sensitivity analysis of the HYPE model parameters using Brogonov’s Delta Moment-Independent Analysis (Brogonov, 2006) is performed to determine the most sensitive parameters of HYPE. These parameters are calibrated to obtain model performance of Kling-Gupta Efficiency (KGE, Gupta et al., 2009) = 0.66, Percentage bias (PBIAS) = 3.14 for streamflow, and PBIAS = -0.03 for TN concentration at the basin outlet for the calibration period. The simulated TN concentration is taken as the initial TN concentration for the study, and the long-term annual mean TN concentration at the outlet of the calibrated model is 4.963 mg/l. The description of the measures, their level of implementation, modification of relevant HYPE files, and parameters that are changed to implement the measures are listed in Table 3.1. The measures are implemented at the beginning of the simulation, and their effect is evaluated after a two-year warm-up period for six years. Nine measures under four categories are provided to the algorithms to distribute in the basin. A condition to not repeat the measure from the same category is applied to ensure no reiteration of a measure in policy development.

Table 3.1 Mitigation measures to reduce TN and their level of implementation in HYPE

| Category | Description | Parameter(s) | File | Level of implementation |
|----------|---|-------------------------------|---------------------|-------------------------|
| I | A. 30% Reduction in amount of N in fertilizer | fn1; fn2 | | |
| | B. 10% Reduction in amount of N in fertilizer | fn1; fn2 | | |
| II | A. 30% Reduction in amount of N in manure | mn1 | CropData.txt | crop |
| | B. 10% Reduction in amount of N in manure | mn1 | | |
| III | A. Tillage using Harrow tines cultivator | fdown1; mdown1; mdown2; | | |
| | B. No-tillage | | | |
| IV | A. 100% efficiency of STP to remove TN | ps_tnconc | PointSourceData.txt | sub-basin |
| | B. 20% increase in efficiency of STP to remove TN | | | |
| | C. 50% increase in efficiency of STP to remove TN | | | |

The objective function of the study is defined as follows:

$$\max f(C) = \frac{\sum_{i=0}^n \bar{x}}{n} - \frac{\sum_{i=0}^n \bar{y}(C)}{n} \quad (3.1)$$

$$i = 1, 2, \dots, n$$

where $f(C)$ is the long-term annual mean TN reduction achieved by C , \bar{x} is the annual mean TN concentration at the outlet of the calibrated model, \bar{y} is the annual mean TN concentration at the outlet of the model achieved by C , C is the combination of measures from the four categories and their respective levels of implementation, and n indicates the years of simulation.

3.2.2 Ant Colony Optimization (ACO)

ACO is inspired by the foraging behavior of ants using stigmergy. When the ants search for food, the initial path taken by an individual ant is essentially random. Once the ants find a food

source, they deposit pheromones to indicate a favorable path for other colony members to follow. When another ant encounters the path during its search, it will most likely follow an existing pheromone trail and enforce the path with its pheromone deposition. Thus, increasing the probability of other ants selecting the specific path. The shortest path will have a higher pheromone deposition than the longer path and attracts more ants. In this way, ants can find the shortest path to food sources using pheromone information (Dorigo and Stützle, 2004).

In the optimization technique, the colony of artificial ants is equipped with heuristic information and knowledge of searching for optimal solutions in the decision space. They communicate indirectly using pheromones. Pheromones are evaporated over time to avoid ants being stuck at the local optima. Multiple methods of pheromone updating are prescribed by researchers (Dorigo et al., 1996; Bullnheimer et al., 1997; Stützle and Hoos, 2000). In this study, pheromone update is done per the MAX-MIN ant system (MMAS, Stützle and Hoos, 2000) as it has proven to be the best performing variant of the Ant System (Dorigo and Stützle, 2004).

Adaptation to the spatial distribution

Figure 3.2 demonstrates the ACO process adopted in this study. In optimizing the spatial distribution of mitigation measures, the objective function is to maximize the TN reduction at the basin outlet. Along with the measures and their level of implementation, the algorithm is initialized with a maximum number of iterations (*iterMax*), number of ants (*antNo*), heuristic information (η), evaporation rate (ρ) and initial pheromone concentration (τ_0).

In the first step, an artificial ant randomly selects a measure and its level of implementation. The pair is implemented in the hydrological model HYPE, and the resulting TN reduction is calculated. The next pair is selected based on probability, which is dependent on the pheromone trail (τ_{SL}) and heuristics information (η_{SL}).

The transition probability ($P_{SL}^k(iter)$) for k^{th} ant to select the next pair (SL) is defined as:

$$P_{SL}^k(iter) = \frac{[\tau_{SL}^{iter}]^\alpha [\eta_{SL}^{iter}]^\beta}{\sum [\tau_{SL}^{iter}]^\alpha [\eta_{SL}^{iter}]^\beta} \quad (3.2)$$

where τ_{SL}^{iter} is the value of the pheromone trail in the current iteration $iter$, η_{SL}^{iter} is the heuristic function (individual TN reduction), α is the pheromone exponential parameter, and β is the desirability exponential parameter.

At each iteration $iter$, the pheromone trail is updated according to MMAS (Stützle and Hoos, 2000) as follows:

$$\tau_{SL}^{iter+1} = \rho * \tau_{SL}^{iter} + \Delta \tau_{SL}^{best} \quad (3.3)$$

where ρ is the pheromone evaporation rate, $\Delta \tau_{SL}^{best} = f(s^{best})$, and $f(s^{best})$ is the solution achieved by either the iteration-best ant (s^{ib}) or the global-best ant (s^{gb}) depending on $iter$ value.

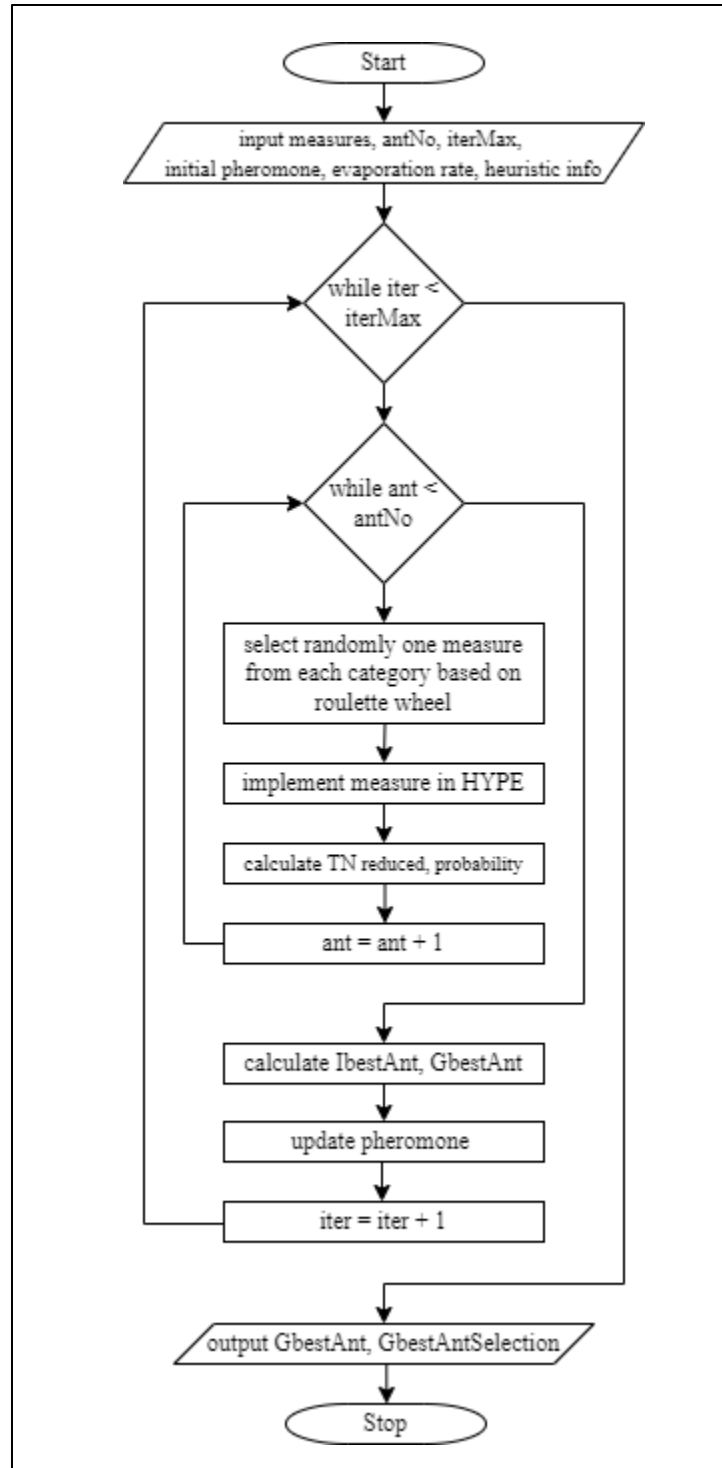


Figure 3.2 Flowchart of Ant Colony Optimization for spatial distribution of measures

According to Stützle and Hoos (2000), the use of either s^{ib} or s^{gb} solution in the pheromone update ensures a more vigorous exploration of the search space in the earlier iterations and more vigorous exploration of the overall best solution during the later iterations. And to avoid stagnation of the search range of pheromones, explicit limits are placed on pheromone trails such that,

$$\tau_{min} \leq \tau_{SL}^{iter} \leq \tau_{max} \quad (3.4)$$

where τ_{min} is the minimum τ value and τ_{max} is the maximum τ value. In this study, the minimum τ value is assigned 0, while the maximum τ value for an iteration is calculated using the following equation:

$$\tau_{max}^{iter} = (1 - \rho) * f(s^{gb}) \quad (3.5)$$

where $f(s^{gb})$ is the solution achieved by the global-best ant. At the end of the optimization, the final selection of the ants forms an optimal spatial distribution of mitigation measures and their level of implementation. Detailed information on ACO and MMAS can be found in Dorigo and Stützle (2004).

3.2.3 Particle Swarm Optimization (PSO)

PSO is inspired by the social behavior of a school of fish or flock of birds to find food or shelter (Kennedy and Eberhart,1995). The birds or fish (particles) base their search on the knowledge of their own experience and the swarms' experience. Thus, the entire swarm reaches the destination at a quick pace. According to Kennedy and Eberhart (1995), the particles are assigned initial location and velocity in the optimization technique. Each particle determines the best location depending on the evaluation of the objective function. New velocities are computed based on the current velocity, particle's best location so far and swarm's best location so far. The next location is iteratively computed based on the current location and the new velocity.

Adaptation to the spatial distribution

Figure 3.3 demonstrates the PSO process adopted in this study. Similar to ACO, PSO is also initialized with the maximum number of iterations ($iterMax$) and the number of particles (pNo). In the first step, particles are initialized with a combination of a random measure and their level of implementation. These measures are implemented in HYPE, and the resulting TN

reduction is calculated. The best selection of a pair by the particle so far ($IbestP$) and the swarm's best selection of pair so far ($GbestP$) are calculated. The velocity of a particle for the next iteration, V_{SL}^{iter+1} , is computed as follows:

$$V_{SL}^{iter+1} = w * V_{SL}^{iter} + c_1 * r_1 * (IbestP_{SL} - P_{SL}) + c_2 * r_2 * (GbestP_{SL} - P_{SL}) \quad (3.6)$$

where w is the variable inertia weight, V_{SL}^{iter} is the velocity of the particle in the current iteration, $iter$, c_1 and c_2 are the cognitive and social parameters of the particle (in this study, $c_1 = c_2 = 2$ is used (Ozcan and Mohan, 1999)), r_1 and r_2 are the random numbers, $IbestP_{SL}$ is the best selection by the particle so far, $GbestP_{SL}$ is the swarm's best selection so far, P_{SL} is the current selection. The value w is computed using the formula given by Shi and Eberhart (1999),

$$w = (w_1 - w_2) \frac{iterMax - iter}{iterMax} + w_2 \quad (3.7)$$

where $iterMax$ is the maximum number of iterations, $iter$ is the current iteration and the values of w_1 and w_2 are 0.9 and 0.4, which is widely accepted by researchers for PSO applications (Jordehi and Jasni, 2013). The following equation calculates the next pair:

$$P_{SL}^{iter+1} = P_{SL} + V_{SL}^{iter+1} \quad (3.8)$$

where, $P_{SL}^{(iter+1)}$ is the selection of pair for the next iteration, P_{SL} is the current selection, $V_{SL}^{(iter+1)}$ is the velocity of a particle for the next iteration.

Thus, to seek the optimal solution, each particle derives its next selection from its previous best ($IbestP$) selection and the swarm's best ($GbestP$) selection. At the end of the optimization, the final selection of the particles forms a selection of optimally distributed mitigation measures and their level of implementation. A penalty function is introduced to ensure the search of particles stays within the feasible region. A reduction of 0.01 in the solution achieved by the particle is applied, and the particle is randomly assigned the next pair.

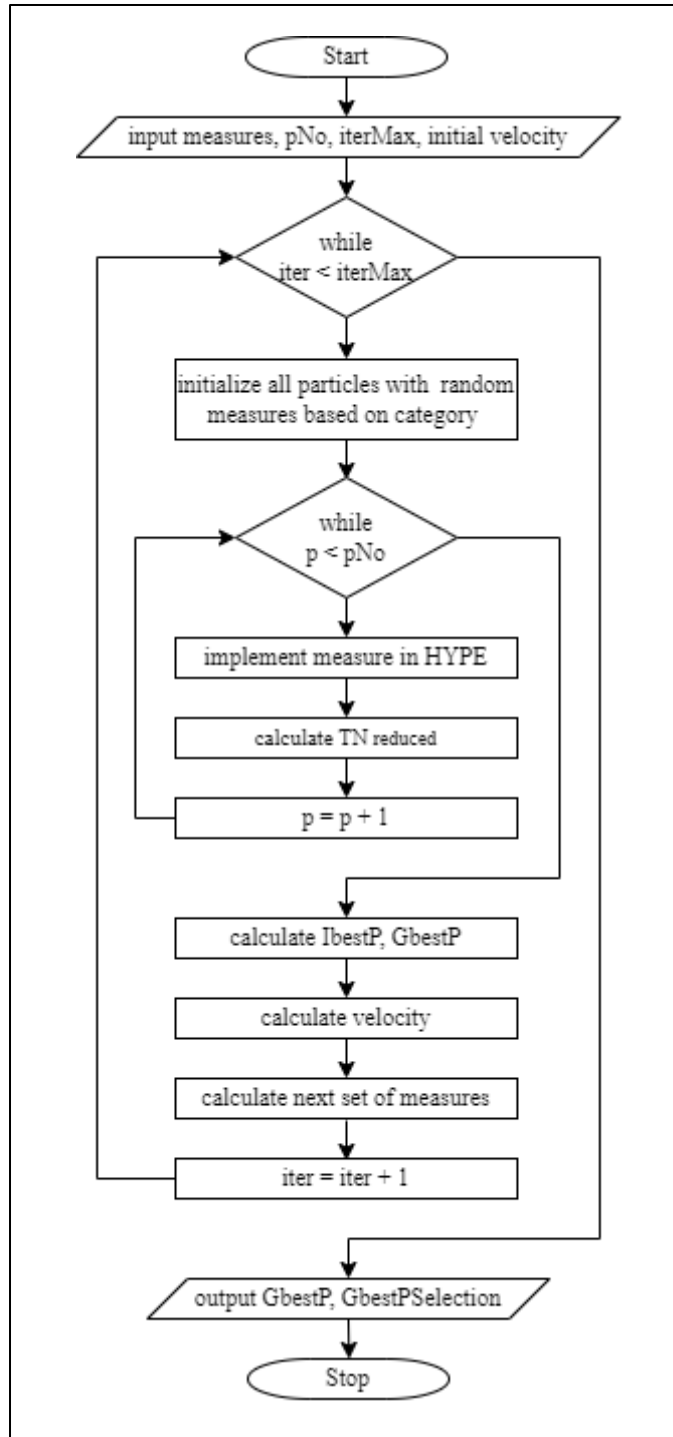


Figure 3.3 Flowchart of Particle Swarm Optimization for spatial distribution of measures

3.3 Results and Discussion

3.3.1 Parameter selection

In this study, ACO is parameterized by α , β , ρ , number of ants and maximum iteration. Since the approach used in the optimization of the water distribution network is similar to the one used in this study, the values of $\alpha = 1$, $\beta = 0.5$ and $\rho = 0.98$ from Zecchin et al. (2003). The algorithm was run for 100 iterations with a varied number of ants (10, 20, 30, 40, 50). It can be seen from Table 3.2 that even with only 10 ants, the global best solution achieved by the ACO is on par with those achieved by a higher number of ants. The difference lies in the computational time required to run a larger number of ants to accomplish the best solution. Similar results can also be seen for PSO when the algorithm is run for 100 iterations with 10, 20, 30, 40, and 50 particles. The number of ants selected for ACO is 10, and 30 particles are selected for PSO.

Table 3.2 Results for ACO and PSO

| Number of ants/particles | ACO | | PSO | |
|--------------------------|--------------------------|------------------|--------------------------|------------------|
| | Global best solution (C) | Iteration number | Global best solution (C) | Iteration number |
| 10 | <u>0.907</u> | <u>57</u> | 0.904 | 13 |
| 20 | 0.905 | 66 | 0.905 | 20 |
| 30 | 0.907 | 38 | <u>0.906</u> | <u>7</u> |
| 40 | 0.907 | 18 | 0.906 | 29 |
| 50 | 0.905 | 12 | 0.905 | 66 |

3.3.2 Spatial distribution of mitigation measures

The measures selected by ACO and PSO are shown in Table 3.3. The maximum long-term annual mean TN reduction achieved by ACO is 0.907 mg/l (18.26 % reduction), while PSO achieved 0.906 mg/l (18.25 %). In this study, we see that both algorithms are on par with slightly better performance by ACO.

Table 3.3 Measures selected by ACO and PSO

| Algorithm | Selection (level, measure) |
|------------------|---|
| ACO | [(5, IA), (1, IIA), (1, IIIB), (1015, IVA)] |
| PSO | [(5, IA), (5, IIB), (1, IIIB), (1015, IVA)] |

The crop-level measures chosen by ACO and PSO can be visualized in Figures 3.4 and 3.5, respectively. The final set of measures selected by ACO includes,

- i) 100% efficiency of sewage treatment plants at subbasin 1015 (Kläranlage Salzgitter-Nord) to reduce TN,
- ii) reduce 30% of N fertilizer application from the current application level in the sugarbeet fields (Category I),
- iii) reduce 30% manure application from the current application level in the winter wheat fields (Category II), and
- iv) adopt no-tillage (100% reduction in tillage) in the winter wheat fields in the basin (Category III).

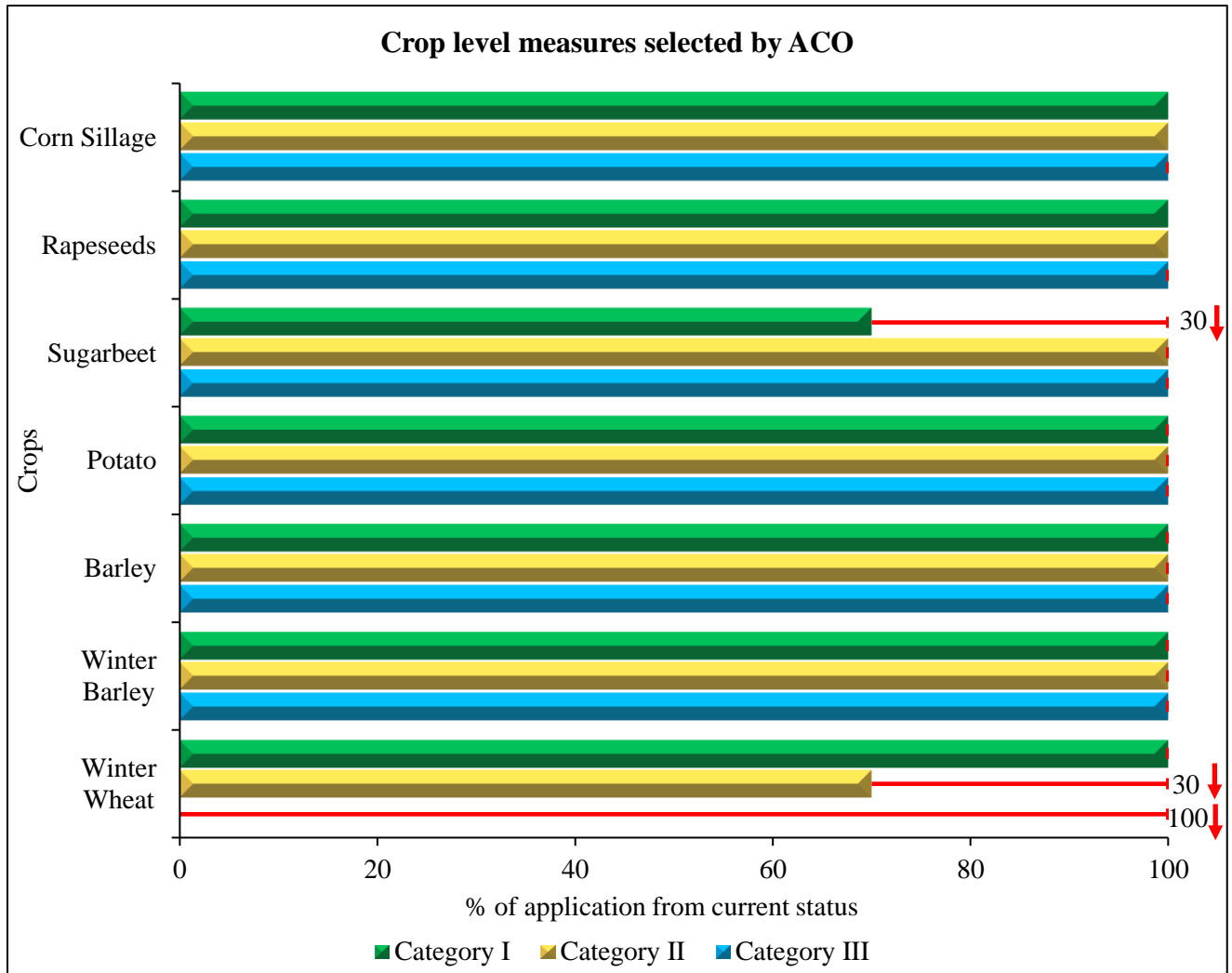


Figure 3.4 Selection of crop-level measures by ACO (downward arrow indicates reduction)

The final set of measures selected by PSO includes,

- (i) 100% efficiency of sewage treatment plants at subbasin 1015 (Kläranlage Salzgitter-Nord) to reduce TN,
- (ii) reduce 30% of N fertilizer application to sugarbeet fields from the current application level (Category I),
- (iii) reduce 10% of manure application to sugarbeet fields from the current application level (Category II), and
- (iv) adopt no-tillage (100% reduction in tillage) in winter wheat fields in the basin (Category III).

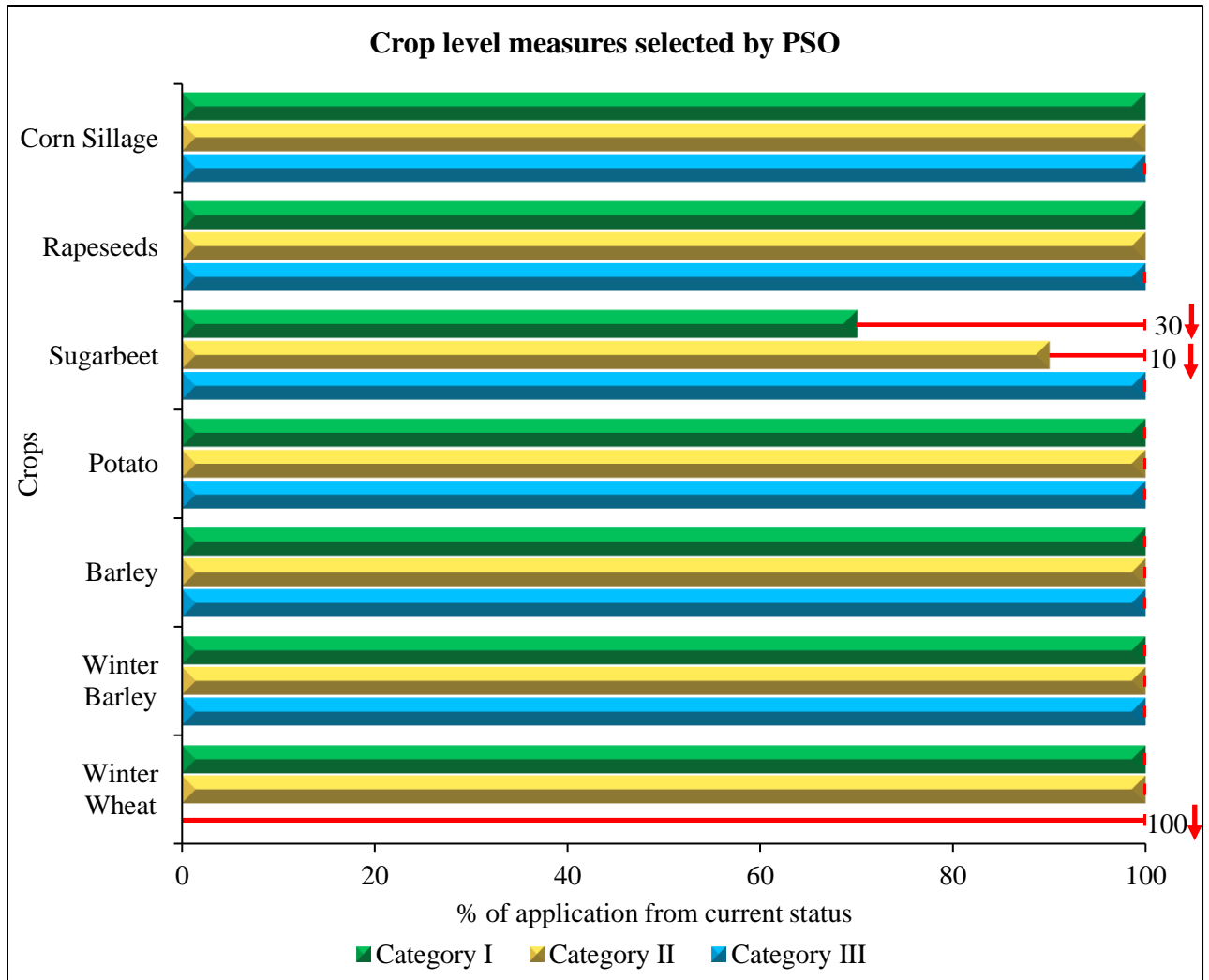


Figure 3.5 Selection of crop-level measures by PSO (downward arrow indicates reduction)

The annual reduction achieved by the measures selected by the algorithms is compared with the initial annual mean TN concentration at the Peine gauging station. As seen in Figure 3.6, both algorithms are on par with each other and successfully reduce total nitrogen concentration at the basin outlet. Both algorithms achieved a maximum annual mean reduction of 1.18 mg/l of TN for 2011, while the minimum annual mean reduction of 0.53 mg/l of TN in 2007 in terms of absolute value. The maximum percentage reduction of annual mean TN was achieved in 2008 (31%), and the minimum percentage reduction of annual mean TN was achieved in 2010 (11%).

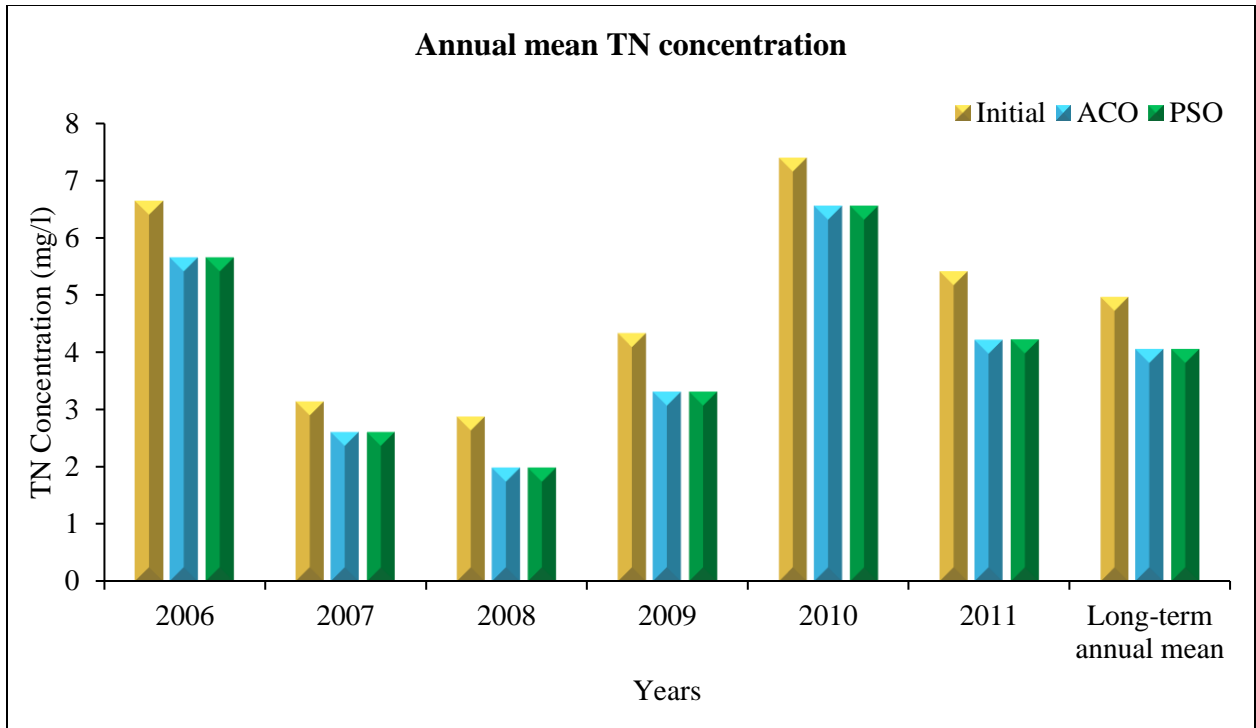


Figure 3.6 Annual mean TN achieved by ACO and PSO

The effects of implementing the measures chosen by ACO and PSO on river reaches in long-term annual mean TN percentage reduction are shown in Figures 3.7 and 3.8, respectively. The reach in subbasin 15 shows the highest reduction (43.8%) by both algorithms, indicating the high contribution of TN by the wastewater treatment plant. The subbasins downstream of 15 – 14, 13, 11, 09 and 07 also show a substantial reduction in long-term annual mean TN of greater than 10%. Other critical reductions can be seen in subbasins 06, 10 and 12 for both algorithms. A detailed table with the reduction achieved by the algorithms for each reach in a subbasin is provided in Appendix B.

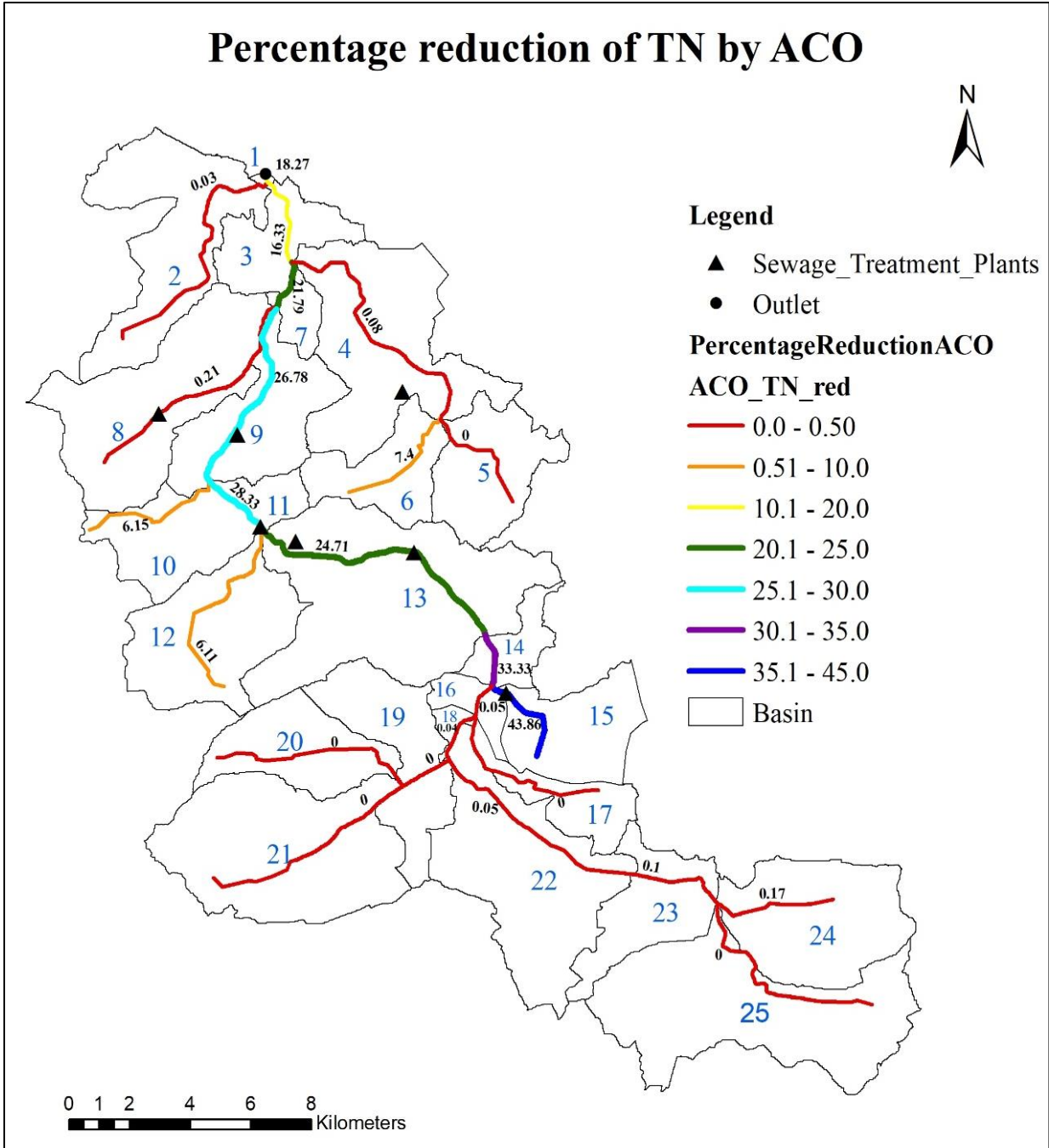


Figure 3.7 Long-term annual mean percentage reduction of TN by ACO

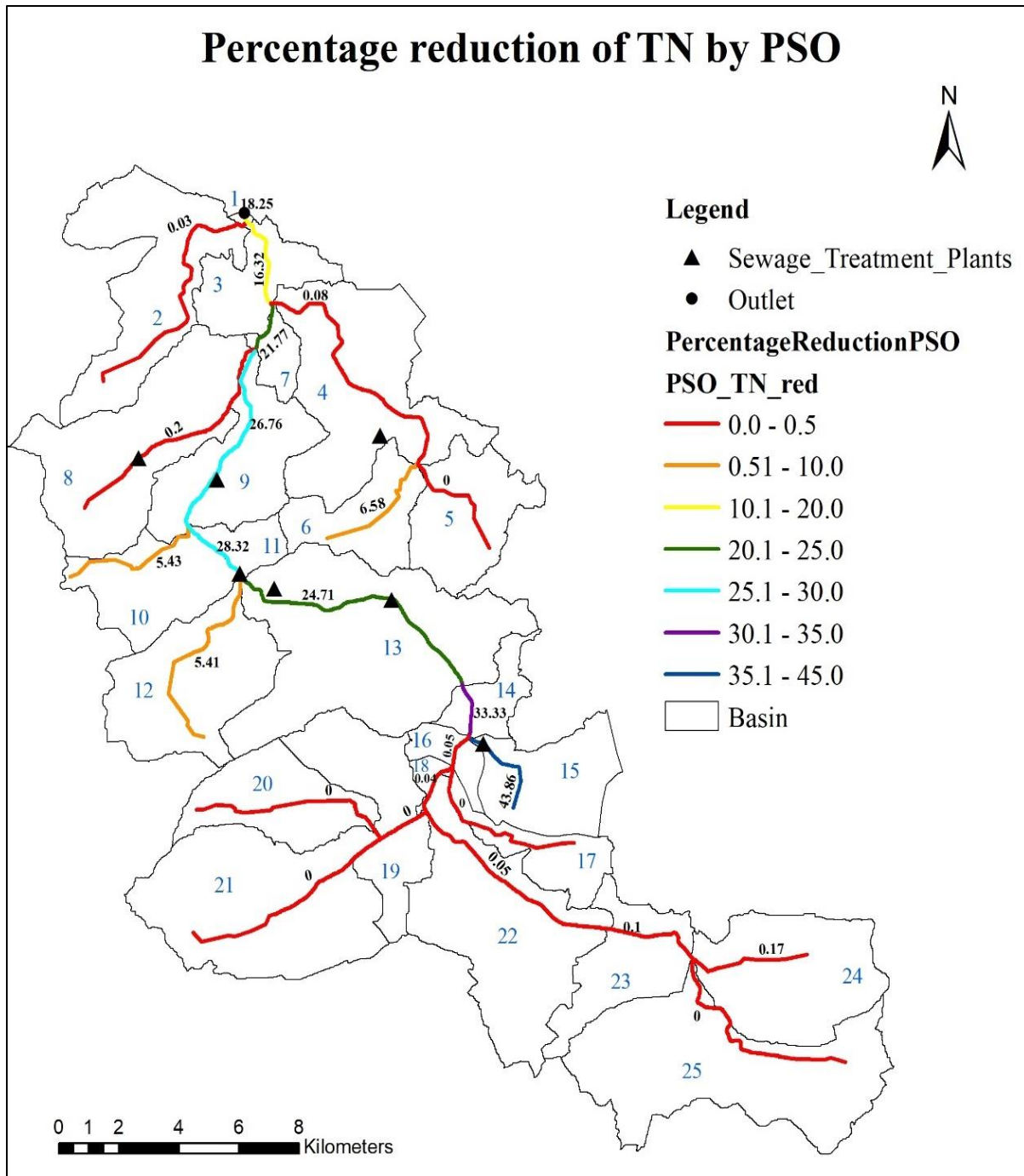


Figure 3.8 Long-term annual mean percentage reduction of TN by PSO

A binary map to indicate the reaches on which ACO achieved slightly better long-term reduction than PSO is shown in Figure 3.9. The orange-colored reaches indicate better performance by ACO, while blue-colored reaches indicate the same performance by both algorithms. Better spatial performance of ACO over PSO can be seen.

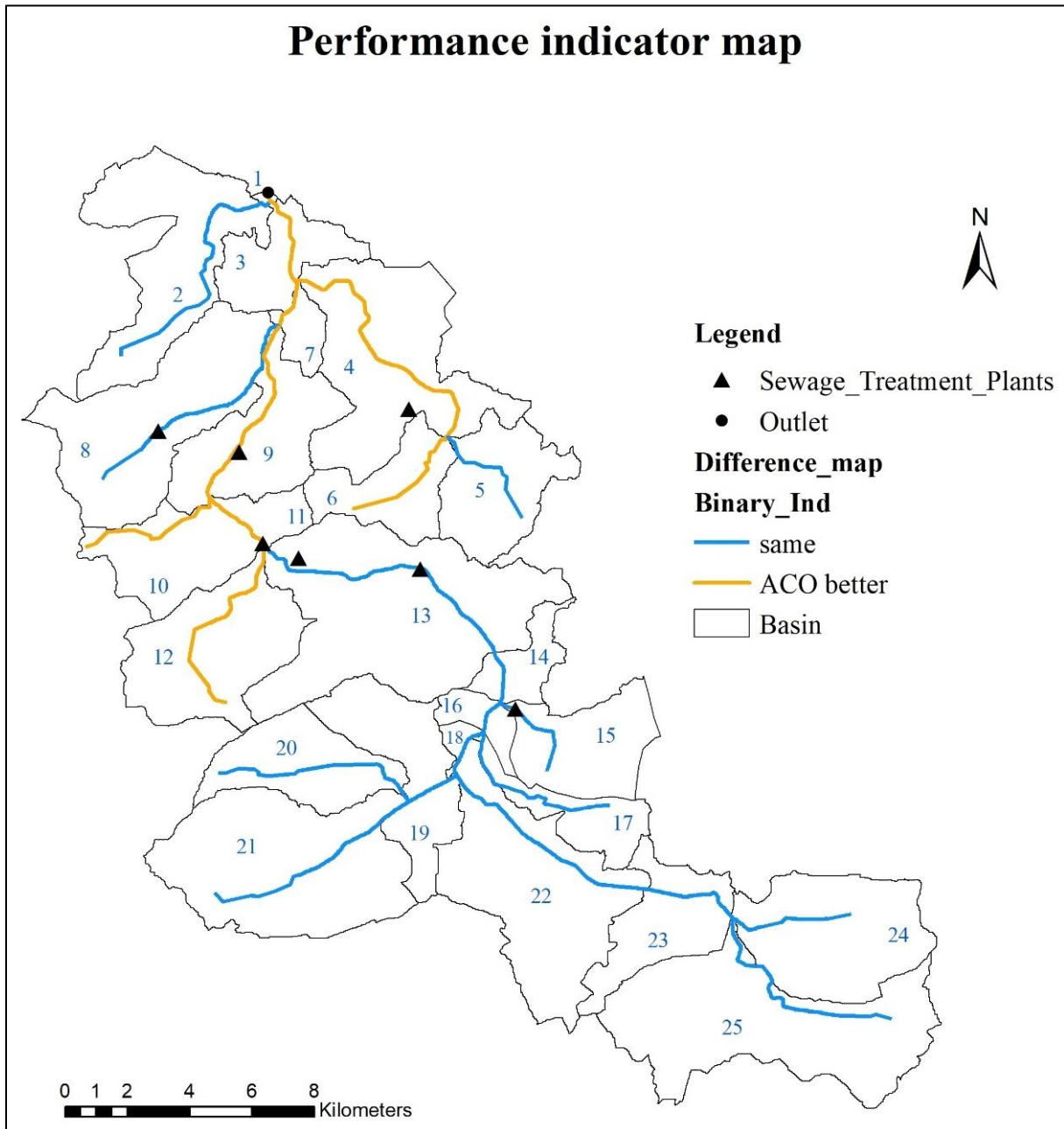


Figure 3.9 Performance indicator map

3.4 Conclusions

This research explores the application of ACO and PSO to distribute the mitigation measures in a river basin spatially. Both algorithms can distribute measures in the river basin to achieve long-term TN reduction. The reduction achieved by the algorithms is similar to each other though the measures selected by them slightly vary. Provided that the implementation of multiple measures at various sub-basins forms a strategy, the solution generated by the algorithm may yield more than one strategy as optimal strategy. In such cases, it is the discretion of the decision-makers to choose what works best for their basin conditions.

This study indicates the forte of bio-inspired algorithms in selecting measures and distributing them on multiple implementation levels. ACO and PSO are able to achieve an 18.26 % and 18.25 % reduction of long-term annual mean TN concentration at the outlet of the basin, respectively. The considered algorithms have high practical significance as they are reliable, simple and can be easily implemented for solving problems on a basin-scale by optimizing integrated river basin management plans. ACO contains a mixture of descriptive procedures and equations, while PSO is mainly based on dynamic velocity equations (Yang et al., 2018). To guarantee the particles stayed within the feasible region, a penalty function had to be used for PSO, while ACO did not require a penalty function.

Basic algorithms of ACO and PSO are used in this study to optimize the spatial distribution of mitigation measures to indicate the ability of bio-inspired algorithms in IRBM. In future works, it is highly recommended to consider the application of bio-inspired algorithms with parallelization, integration with local search operators and hybridization with other bio-inspired algorithms like GA. Also, with respect to problem formulation, a single objective function is used in this study, i.e., maximum reduction of long-term annual mean total nitrogen concentration. In future works, it is recommended to use multi-criteria, multi-constraints problems with social acceptance, and ecological significance, which is closer to real-world application.

The hydrological model HYPE was chosen in this study because of its low computational cost. However, to evaluate the effects of measures in detail across the subbasins and assess the emission and immission aspects within the basin, future studies can use a comprehensive agro-hydrological model, urban hydrological model and crop models. Future studies can also include daily data of

discharge and TN concentration from wastewater treatment plants and continuous long-term series of observed TN concentration, and actual data of fertilizers applied in the fields. Other mitigation measures like hydro-morphological mitigation measures, implementation of buffer strips, use of catch crops and crop rotation schemes can also be analyzed to achieve higher reduction.

The spatial distribution of measures helps the decision-makers evaluate the extent to which such measures effectively reduce the total nitrogen concentration in surface waters. However, a comprehensive understanding of the spatial restrictions and conflicts in implementing the measures like intertwined objectives should be evaluated too. They will differ from basin to basin based on the local ecological, socioeconomic status, and stakeholders, and therefore, each catchment needs to be evaluated separately.

4. Application of the theory of planned behavior with agent-based modeling for sustainable management of vegetative filter strips

This chapter is an edited version of Kasargodu Anebagilu, P., Dietrich, J., Prado-Stuardo, L., Morales, B., Winter, E., Arumi, J. L. (2021). Application of the theory of planned behavior with agent-based modeling for sustainable management of vegetative filter strips. Journal of Environmental Management 284, 112014.

Abstract

This study proposes an innovative socio-hydrological modeling framework for the development of environmental policies that are tailored to farmers' attitudes and economic interests but also optimize environmental criteria. From a farmers' on-site survey, a behavior model is developed based on a modified Theory of Planned Behavior (TPB). The dynamics of the social and environmental system are implemented by coupling an agent-based model (ABM) with an agro-hydrological model for vegetative filter strips (VFS). A case study is conducted with farmers from the Larqui river basin, Chile, to understand their standpoint on VFS to reduce soil loss in their agricultural fields and protect water bodies. Partial least square structural equation modeling is used to analyze the survey on farmers' aspirations and attitudes. It showed that the constructs added to TPB (behavioral morality, behavioral willingness, knowledge) had a significant effect on modeling the intention and behavior of farmers to have VFS. Based on the survey, the farmers were categorized into perceptive, proactive, bounded rational and interactive agents. An ABM was developed using the behavioral categorization, related decision rules, and utility functions of agricultural activities, including the VFS implementation and management. The results of the ABM corroborate with the survey of the farmers. The survey supports the view that the decision on the width of VFS is not solely dependent on the utility generated and the reduction in soil losses but also on the behavior of farmers. This behavioral sociohydrological modeling framework is capable of supporting policy-makers in developing tailored environmental policies that might improve the acceptance of sustainable agricultural practices by farmers.

Keywords: Agent-based modeling, Theory of planned behavior, Vegetative filter strip, NetLogo, Socio-hydrology, Farmer survey.

4.1. Introduction

In environmental management, the interplay between humans and natural resources is a dynamic system of natural processes and human behavior under institutional and legal boundaries. Environmental management does not only integrate different disciplines but focuses on the interface between humans and nature. The emerging research in socio-hydrology is an example of water resources management (Sivapalan et al., 2012; Di Baldassarre et al., 2015). Coupling human behavior with economic and environmental models is essential in order to develop tailored policies for stakeholders (Jager et al., 2000; Allred and Gary, 2019; Granco et al., 2019; Dessart et al., 2019). In the agricultural sector, there is extensive research on the adoption of technological and environmental innovations, and several tools support the evaluation of their impacts on livelihoods and the environment (Berthet et al., 2016; Llewellyn and Brown, 2020).

Vegetative filter/buffer strips (VFS) are natural or managed structures at the interface between agricultural land and water bodies. VFS provides multiple benefits and is thus considered an effective environmental management measure (Lovell and Sullivan, 2006). They remove sediments and pollutants from overland flow (Dillaha et al., 1989; Deletic and Fletcher, 2006), stabilize streambanks (Dosskey et al., 1997), conserve wildlife habitats (Boulet et al., 2003), provide extra yield if they can be harvested (Borin et al., 2010), and they add aesthetic value to the field (Klein et al., 2015). Lowerance et al. (2002) and Abu-Zreig et al. (2004) reported sediment removal of up to 97% in a well-maintained VFS. VFS reduced runoff volume up to 90%, sediment up to 94%, nitrate concentration by 88% and phosphate concentration by 95% (Saleh et al., 2017). The trapping efficiency of VFS is majorly influenced by their width (Abu-Zreig, 2001; Akan and Atabay, 2016; Campo-Bescos et al., 2015). The effects of VFS policies, including regulations about their width, need to be examined at the farm and catchment level (Dosskey et al., 2008).

Chile recommends the use of VFS to prevent the movement of eroded soils into nearby waterbodies. However, the use of VSF is only mandatory for forest plantations (Romero et al., 2014) and voluntary in the case of animal farms depending on their environmental licenses (Flores et al., 2010). There is no particular directive for the implementation or protection of VFS in agricultural fields. Developments in other countries show that riparian areas have been converted for crop production with the consequence of conflicts between farmers and environmentalists. Often, measures were later done to restore at least a small VFS. This study investigates if the

interplay between the attitudes and behavior of farmers, on the one hand, and the natural environment, on the other hand, can be described by a coupled system of a VFS model and an agent-based model (ABM) based on the social theory of planned behavior.

Studying and understanding human behavior is important to comprehend, develop and improve decision-making processes. Neoclassical decision theory assumes that rational actors introduce new technology when the benefits exceed the costs of introduction and that relative prices determine the optimum in the new equilibrium. Simon (1957) extended decision theory with behavioral aspects by introducing the ‘satisficing concept’ as a base of a new ‘bounded rationality’ paradigm, which accepts compromise solutions for complex decision problems rather than search for optimum solutions. Recent theories consider psychological and sociological factors that influence decision-making behavior, namely aspirations, risk attitudes, cultural norms and peer group influence (Kahneman, 2003; Weersink and Fulton, 2020). While humans have different individual thinking and behavioral processes, societal and environmental elements also influence decision-making (Miyasaka et al., 2017). Schulze et al. (2017) classified the most influential factors of a human decision-making model as monetary returns, social groups, impact on others, environmental altruism, and environmental/ non-economic benefits such as aesthetic values or recreation. Human responses with respect to policies that recommend field-level changes require multi-disciplinary knowledge and understanding of not only the policy and the effects of it on the environment but also the effect of the policy’s outcome on stakeholders like farmers (Smajgl et al., 2011).

In 1991, Ajzen developed the Theory of Planned Behavior (TPB) as a successor to the Theory of Reasoned Action by Fishbein and Ajzen (1975). He theorized that the likeliness to perform a behavior stems from the strength of the intention and willingness to try and exert effort towards the task at hand (Ajzen, 1991; Suh and Hsieh, 2016). According to TPB, the intention to perform is dependent upon attitude, subjective norms and perceived behavioral control. The simple and efficient framework of TPB makes it easier to analyze behavior from the background information collected on-site in the form of local interactions or in-depth surveys (Russo et al., 2015).

Zubair and Garforth (2006) have studied farmers’ behavior to different aspects related to adopting agroforestry practices using TPB. They concluded that TPB provides a structural

framework to identify the outcomes based on beliefs, social interaction and behavioral control factors. Cooper (2017) evaluated the application of TPB to ensure compliance with urban water restrictions and concluded that behavioral compliance is significantly influenced by the constructs - attitude, social norms and behavioral control as explained by the TPB model. Caffaro et al. (2019) assessed different paths using which the information environment affects the adoption of sustainable measures by the farmers based on the TPB constructs. They concluded that attitude and perceived behavioral control were the dominant constructs that influenced farmers' behavior. The farmers' decision was not influenced by subjective norms in that study. Understanding the different aspects of behavioral theory can give an insight into the decision-making process of the farmers, capturing different dynamics and feedbacks as seen in a socio-ecological system (Liu et al., 2008; Allred and Gray, 2019). Due to the presence of clarity of constructs and correlational confirmation (Skår et al., 2008), TPB is used in the current study.

Agent-based models (ABM) emulate the internal behavior of agents in a system, their interaction amongst each other, as well as their interaction with the environment. Enrico Fermi, a physicist in the 1930s, incited upon the concept of ABM whilst trying to transport neutrons through matter (Turrell, 2016). However, the very first economic ABM was developed to analyze agents' preference for the location to live by Schelling (1971). The agents and their environment are represented explicitly in ABM, thus modeling local interactions in a straightforward manner (Izquierdo et al., 2019). Internal conditions for behaviors can also be encoded to express real-world conditions (Matthews et al., 2007). The ability of ABM to be analogs of real behavior makes it suitable to model the heterogeneous and complex structure of socio-environmental and socio-hydrological systems. The agent's behavior is modeled using the knowledge extracted from the context information without the use of training datasets. ABM is considered as a decision support tool through which, in an environment, an agent's interaction is simulated, which would be expensive to analyze in the real world (Castilla-Rho et al., 2015).

Although the application of ABM was initially used in computer simulations (An, 2012), in recent years, ABM is applied to diverse studies. ABM has been applied for studies involving the farmers' behavior with respect to the application of landscape, economics (Guillem et al., 2015), environmental effects (Heckbert et al., 2010), socio-hydrology (Pouladi et al., 2019), and policy development (Happe et al., 2006; Brady et al., 2012; Granco et al., 2019). One of the

prominent merits of using ABM is to deal with public involvement in the representation of scientific formulations in the form of ‘soft sentences’ that is comprehensible and easily understood by all the stakeholders (Rixon et al., 2007). Rounsevell et al. (2012) discuss the suitability of ABM with qualitative social-survey data. According to Etienne et al. (2002), the analysis of different viewpoints for representing the agent’s perception is important in their simulation to encourage the agents to act collectively. Sengupta et al. (2005) investigated the acceptance of a conservation program by farmers to avoid the cultivation in endangered land due to erosion in exchange for monetary value. The ABM developed in their study is combined with a geographical information system to provide spatial effects of land use policies which are then used in decision-making with the help of a decision tree. Some case studies where an agent-based simulation model has been used in environmental studies have been documented by Hare and Deadman (2004). Therefore, ABM is chosen to be adopted in this study to model farmers’ decision-making process in the economic, social and environmental context.

The overall aim of this work is to demonstrate the importance of developing coupled social and technical models based on social behavioral theories when investigating human-environment feedbacks. For this, we follow these main objectives:

- (a) Development of a model of farmers’ behavior under the social and environmental influence by an empirical survey and an extension of the TPB;
- (b) Investigation of environmental and social factors that motivate farmers to keep or implement a certain width of VFS by coupling a VFS model and an ABM;
- (c) Discussion of implications for effective agricultural and water policy-making based on results from a case study in Chile.

4.2. Materials and methods

4.2.1. Study area

This study has been carried out in the district of Diguillín, which is part of Región de Ñuble in Chile. It has a flat topography with an elevation range of 65–163 m.a.s.l. The catchment is in the upstream of River Larqui between Latitude 36°41’ – 36°48’ S and Longitude 72°16’ – 72°06’ W. The basin has an area of 101 km². River Larqui receives water from the nearby streams and

flows into River Itata. It receives an annual average rainfall of 1000 mm, and the mean temperature varies from 20°C in summer to 7°C in winter. Volcanic soil is predominant in the region leading to the formation of fertile Bulnes soil (red clay-loam) majorly in the basin. The basin shows strong agricultural activity, mainly based on annual crops, sugar beet, orchards along with meadows, thickets, forests and livestock. The basin experiences soil erosion, reduced crop yields and increased cost of production (Flores et al., 2010). Bonilla and Vidal (2011) have revealed that furrow irrigation systems adopted by farmers can also be one of the factors that hike the rate of soil erosion.

According to Centro de Información de Recursos Naturales (CIREN) report (2010), major parts of the study area experience moderate to light erosion. Moderate soil erosion refers to erosion that has exposed the subsoil surface and, in some cases, results in the formation of grooves. Light erosion refers to the loss of soil that occurs on surfaces with slope and semi-dense vegetation cover of 50–75% that would slightly alter the thickness and texture of the soil. Thus, the conservation and management of VFS are suitable measures to tackle erosion and finally reduce sediment transport in the region.

4.2.2. Modeling framework

To understand and model the decision-making process of farmers regarding VFS, a socio-hydrological chain of experiments and models is developed, as shown in Figure 4.1:

- (i) a field survey is carried out with random sampling method to investigate the field conditions and attitudes of a group of farmers belonging to the Larqui river basin;
- (ii) the constructs of the TPB are extended for socio-environmental problems, and the survey is evaluated using partial least squared structural equation modeling (PLS-SEM);
- (iii) decision rules and utility functions are developed to describe farmers' behavior and decision processes based on TPB and monetary benefits from agricultural activities and VFS;
- (iv) an ABM using the NetLogo software is created with decision rules for agents based on their behavioral categorization;

- (v) soil erosion for the full combination of different field classes and widths of VFS is computed by the model VFSMOD-W, the results of which are coupled with ABM to implement human-environment feedbacks;
- (vi) the results of ABM are evaluated, and factors influencing the decision-making of farmers to ensure a certain width of VFS along their fields are examined.

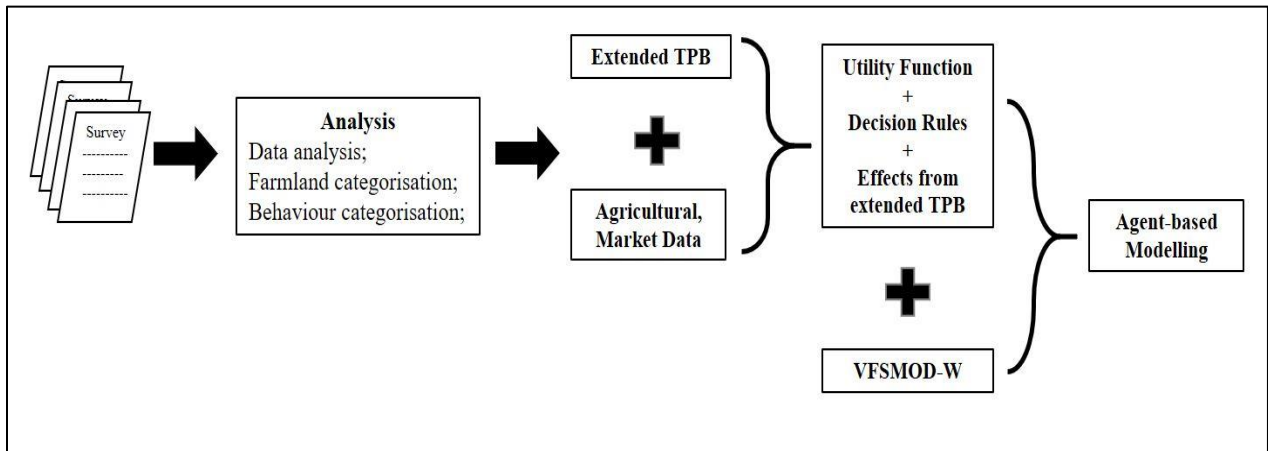


Figure 4.1 Schematic representation of the workflow

4.2.2.1. Field survey and behavioral analysis with an extended TPB

For the survey, a population of 120 farmers was identified, who own farms that are adjacent to River Larqui and are registered with The National Irrigation Commission of Chile (Comisión Nacional de Riego, CNR) as consumers of water from River Larqui at the time when the survey was conducted. A simple random sampling method is adopted to collect the survey of 92 farmers, who agreed to participate in the study. The questionnaire focused on farmers who cultivate crops and vegetables on their land. It is inspired by Armstrong and Stedman (2012). In this study, a five-point Likert scale is used, which allows the farmers to express how much they agree or disagree with a given statement. The survey is designed to gather information on the agricultural practices of the farmers, their perspective on the environment, water resources and vegetative filter strips. The survey includes questions that support the evaluation of different constructs of TPB to analyze the factors influencing the decision-making of the farmers and is part of supplementary material (Appendix C). It is divided into five sections. The first section contains questions to gather basic

information about the agricultural field, like size, layout, the crop grown, and irrigation techniques used, etc. The next sections were divided to address questions related to TPB.

The assumptions used in TPB are that human behavior is goal-oriented, influenced by society and peers, and decisions are made with a logical and rational approach (Ajzen, 1985; Sandberg and Conner, 2008). The constructs of TPB are as shown in Figure 4.2. Ajzen (1991) defined behavioral intention as ‘the amount of effort one is willing to exert to attain a goal.’ The intention is steered by the attitude towards the behavior and subjective norm (Menozzi et al., 2015). Subjective norm refers to societal pressure perceived by an individual on whether to perform or not perform the said act (Bijttebier et al., 2018). It refers to the perception of the ability or difficulty that a respondent may face towards executing the behavior. This may be impacted by previous experiences, information received from peers and friends (Ajzen, 1991). Please refer to Ajzen (1991) for detailed information on the development of the original constructs.

To encompass the overall field situation, an extended TPB is used in this study as shown in Figure 4.2. Along with the constructs from the basic TPB, three additional constructs are used in this study – knowledge, behavioral willingness and behavioral morality that describe individual norms. One of the key factors that influence behavior and decision-making is knowledge (Michie et al., 2008). The construct knowledge enables to understand environmental, VFS related knowledge the respondents have and the influence it has on the decision-making behavior. The knowledge of VFS and its benefits on water, flora, fauna, reduction of sediment and pollutant transport via overland flow and economy of the farmers are usually known only to environmental/agricultural experts and organizations despite VFS being recommended as one of the best management practices. Introducing the construct knowledge is based on the assumption that farmers do not have this knowledge which is crucial for them to decide on the width of VFS in their agricultural fields.

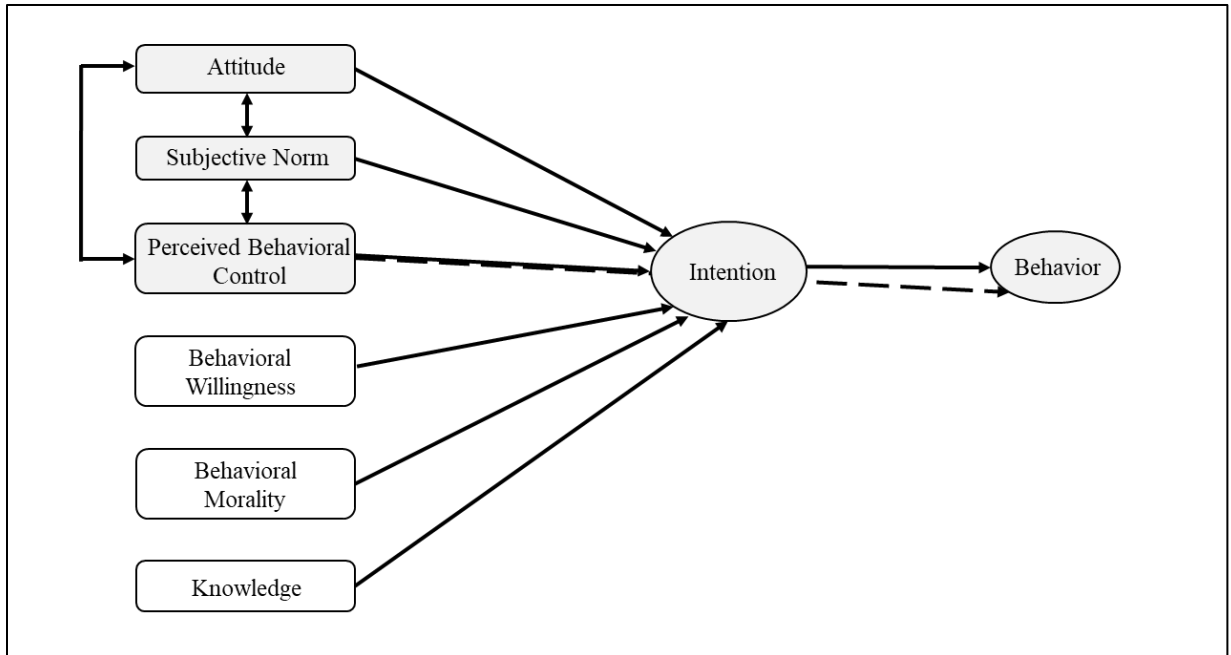


Figure 4.2 Extended Theory of Planned Behavior model

(The original TPB model from Ajzen, 1991 is highlighted with a grey background)

Gerrad and Gibbons (1997) defined behavioral willingness as ‘openness to risk opportunity.’ It entails how far the respondent is willing to enact a particular behavior under certain conditions. In this study, this construct is used to find the influencing factors that would motivate the farmers to overcome the existing prejudice to retain and widen VFS. It is assumed that the influencing factors could be neighbors, association with agricultural organizations, improvements to the environment, an increase of income, monetary compensation, etc. Behavioral morality is another factor that is an integral part of decision-making that has been empirically proven to have a significant effect (Garrigan et al., 2018). With this construct, we attempt to find the thinking of farmers on a personal level about bigger issues of the environment, water, their importance, and protection for the future generation. We try to appeal to farmers’ determination to safeguard the environment on an individual level. With the inclusion of all the different constructs influencing decision-making, an extended TPB, as shown in Figure 4.2, is used in this study. The weights of the constructs of the extended TPB provide information to the policy-makers as to which constructs are most important to ensure the widening widths/keeping VFS in the agricultural fields within the basin.

4.2.2.2. Behavior categorization, development of utility function and decision rules

The farmers are represented as agents in NetLogo with the behavioral change factors implemented in utility functions. The farmers were classified into different types depending on their response to the survey questions to factor in the personality or behavioral category. This classification helps to identify the agents, observe the change in the behavior of the agents, the interaction of the agents amongst themselves and the environment from a socio-economic context. These are important factors as they affect farmers' decision-making (van Dijk et al., 2016). In most of the socio-environmental systems, the agents follow a bounded rational decision or a profit-maximizing decision by taking into account the environmental information. Besides, agents are social learners that imitate other agents (Schlüter et al., 2017). Therefore, the agents in this study are classified as a) **proactive** (having a particular goal to achieve – maximization of profit), b) **perceptive** (pro-environment – cares and is inclined to take actions to safeguard the environment; opt for managed VFS instead of natural), c) **bounded rational** (rational optimizers that act with the limited collected information and also take into account selected neighbor actions) d) **interactive** (communicates with other agents and is easily influenced by neighbor actions). To explain the selection criteria for the different types of agents, the utility function U is defined as,

$$U = P_{UF} + E_{UF} \quad (4.1)$$

P_{UF} represents the monetary benefit from the agricultural activities and E_{UF} represents environmental benefits in monetary terms from having VFS. E_{UF} is further elucidated as,

$$E_{UF} = [L*W](Incentive_{VFS} + B_e) \quad (4.2)$$

The incentive ($Incentive_{VFS}$) received for the width of VFS and saving water resources, the long-term benefit (B_e), which entails the application of nutrients saved and harvest from VFS would vary depending on the length (L) and width (W) of VFS chosen by the farmer. The monetary benefit from agricultural activities, P_{UF} , is further composed of several terms as elucidated in Eq.4.3.

$$P_{UF} = Profit_{AGRI} - Loss_{AGRI} - [L*W] Inv_{VFS} - [L*W] Mt_{VFS} + [L*W] (NP_s + Harvest_{VFS}) \quad (4.3)$$

where $Profit_{AGRI}$ is defined as the profit earned by the farmer from the agricultural field except for the area of VFS, and it is calculated by multiplying the active area (Q) with net income (N) as shown in Eq. 4.4. $Loss_{AGRI}$ is defined as the loss in monetary value caused by soil loss due to erosion, and it is computed Eq. 4.5, where SL is the soil loss, N is the income from agricultural production; C_{SL} is the cost of soil losses. P_{UF} also takes into consideration the loss, which the farmer would face in terms of the initial investment, and the cost of annual maintenance of VFS as well as the financial saving done in terms of nutrients saved by VFS and the financial gaining from harvesting the produce of VFS.

$$Profit_{AGRI} = Q * N \quad (4.4)$$

$$Loss_{AGRI} = SL * N + SL * C_{SL} \quad (4.5)$$

The different parameters and their values in the utility function for this study are listed in Table 4.1.

Based on the behavioral types, different decision-making rules are defined with respect to the utility for future actions. It is factored within decision-making rules that some cases of having of VFS may cause negative utility. Therefore, care is taken to ensure that agents do not accept the economic loss and reject a width of VFS if it has a negative impact on their economic situation. Even the perceptive agents who favor increasing the width of VFS would not go ahead with the width that results in a negative income in any of the three years. All the rules for each type of agent classified are tabulated in Table 4.2.

Table 4.1 Parameters of the utility function

| Parameter | Description | Units | Value | References |
|--------------------------------|---|--------------------------|--------------------------------|---|
| Q | Productive agricultural field | m ² | Variable | From field survey |
| L | Length of VFS | m | according to the field class | FAO, 2017 |
| N | Net income from the agricultural activity | CLP/ yr / m ² | | |
| SL | Soil loss | kg/ yr / m ² | Variable according to the year | From VFSSMOD-W; Tapia and Villavicencio, 2007 |
| CSL | Cost of soil losses | CLP/ yr / kg | | |
| W | Width of VFS | m | [2, 5, 10, 20] | - |
| Inv_{VFS} | Investment cost (one-time) for implementing VFS | CLP/ m ² | 58.4 | Tapia and Villavicencio, 2007 |
| Mt_{VFS} | Annual maintenance cost | CLP/ yr / m ² | 103.3 | Geza et al., 2009 |
| NP_s | Cost of nutrients saved by VFS | CLP/ yr / m ² | 1.79 | Geza et al., 2009 |
| Harvest_{VFS} | Profit from harvesting VFS produce | CLP/ yr / m ² | 6.63 | Artacho et al., 2009; Geza et al., 2009 |
| Incentive_{VFS} | Monetary incentives from the State including water incentives | CLP/ yr / m ² | 15.4 | USDA Program Aid, 2000 |
| B_e | Long-term environmental benefit | CLP/ yr / m ² | 20.67 | |

Monetary units expressed in Chilean Pesos (CLP)

Table 4.2 Decision-making rules for different types of agents

| Type of agent | Basic characteristics | Decision-making Rule |
|------------------|---|---|
| Pro-active agent | Maximize profit | Max U considering $W = 2, 5, 10$ or 20 m |
| Perceptive agent | Favorable to the environment as long as utilities are positive | Case1: $U > 0$; new $U \geq 0$ change W Case2: $U < 0$; decrease W to keep $U > 0$ Case 3: $U = 0$; retain W |
| Bounded rational | Favorable to the environment as long as utilities are better, take into account peer influence as well as information collected | Case1: $U > 0$; new $U \geq U$ change W Case2: $U < 0$; decrease W to keep $U > 0$ Case 3: $U = 0$; retain W |
| Interactive | Decision under peer influence but will ensure utilities stay positive | Case 1: new $U < U$; retain W Case 2: new $U > U$; change W |

4.2.2.3 VFS modeling with VFSSMOD-W

Several models can be used to assess the efficiency and characteristics of VFS. VFSSMOD-W (Muñoz-Carpena et al., 1999) (<https://abe.ufl.edu/faculty/carpena/vfssmod/index.shtml>) was selected in this study, as it requires a limited number of input parameters and can be coupled with the ABM in NetLogo. VFSSMOD-W is an event-based model that simulates infiltration, outflow, and sediment retention efficiency for VFS of different characteristics (Abu-Zreig, 2001; Dosskey et al., 2002). To simulate soil losses with the VFSSMOD-W, a combination of unsteady storm, incoming hydrograph, VFS spatial distribution, and incoming sediment's characteristics have to be introduced. The results of VFSSMOD-W include water outflow, infiltration volume and sediment trapping in the VFS amongst other parameters (Abu-Zreig, 2001). Due to the non-availability of hourly precipitation data, UdeC - Chillán station which is approximately 50 km away from the study area is used. For ease of soil loss simulation and incorporation into the ABM, the agricultural fields of the farmers are divided into 6 classes depending on the area. Accordingly, the source area flow path length (Slength) and source area width (Swidth) are defined for each field class. The slope of the source of the area was considered as 1%.

4.2.2.4 ABM using NetLogo

Modeling the socio-environmental-economic system of how farmers decide on which width of VFS to provide on their farms, depending on the utility incurred by them with active environmental interaction and interaction between the farmers themselves is examined in the current study by an ABM. Each agent represents a farmer who is the owner of a field. Agents are categorized according to their behavioral type as described in 4.2.2.2. A field is represented as one grid cell, independent of the real size of the field. Each tick represents a single day in the simulation period between 1998-2008. It is designed in such a way that; the agents receive information about the soil losses in their fields and the amount of soil retained by the VFS, and the current condition at the end of every year as simulated by VFSMOD-W. An internal parameter (Erosion Problems parameter, EPP) is defined and assigned a value of 1 to indicate that the soil losses in a calendar year are greater than the threshold value, else it is assigned 0. A one-time investment is made by perceptive agents to convert the existing natural VFS into managed VFS based on the knowledge of soil erosion and retention by both managed and natural VFS at the start of the simulation based on the response to the survey.

At the end of every three years of simulation (2000, 2003, 2006 and 2009), the agents are asked to analyze the utility generated, and a decision is made width of VFS for the next three years. This decision is governed by the decision-making rules set for each agent category as described in Table 4.2. During the simulation period, bounded rational and interactive agents are enabled to exchange information via interaction. At the end of the simulation period, the decision of farmers from each category is analyzed to see what width is chosen by them.

Technically, the ABM was implemented in the NetLogo software developed by Uri Wilensky in 1999 (<http://ccl.northwestern.edu/netlogo/>). It is a free and open-source software platform with a simplified and flexible programming language (Castilla-Rho et al., 2015). Hence, it is chosen to be used for the current study. For detailed information, the ODD+D protocol developed by Müller et al. (2013) to describe human decision-making in ABM for the current study is provided in supplementary materials (Appendix C).

4.3. Results and Discussion

4.3.1 Statistical analysis of the field survey and the theoretical model

From the population size of 120 farmers, 92 agreed to participate but 18 farmers did not complete the survey. The resulting sample size of 74 leads to an error margin of 7.1% for the desired confidence level of 95%. The sample size is the upper limit posed by the constraints of the study area and problem, even though a smaller error would be desirable. From the analysis of the survey, it is found that 48% of the respondents reported that they use stream water for irrigation (13%-always; 12%-seasonally; 19%-most of the times; 4% -few days) and more than 50% responded that the water quality ranged between bad to extremely bad based on their observation. However, 95% responded that they had buffer strips on their farm. 72 out of the 74 respondents said they had 'natural' vegetation in their buffer, and only 1 respondent indicated having a manmade buffer strip. Natural buffers are not taken care of or are managed to ensure erosion reduction and the common response for the question as to why they do have it was that 'it is just there'.

Though in the survey it is seen that 54% of the farmers thought that their land is not affected by erosion, this is taken into account as not having knowledge of erosion as erosion is a gradual process. Since the farmers had very little knowledge about buffer strips in general, they had little knowledge about buffer strip programs and how they operate and are beneficial to them. This is seen with 50% of the respondents' replying 'don't know'; 40% agreeing that VFS is beneficial and 9% disagreeing with the benefits of such programs. From the responses provided by the farmers in the survey, the farmers who were motivated only by monetary benefits of VFS are classified into proactive agents (11). The farmers that actively wanted to have VFS in their fields and were concerned about water and environment are classified into perceptive agents (4). The farmers who were aware of the soil erosion in their fields, had knowledge on the quality of water they received and the benefits of buffer are categorized into bounded rational agents (10). The farmers who were willing to have VFS because of their neighbors or friends are categorized into interactive agents (49).

To analyze the causal relationship of the TPB, structural equation modeling (SEM) was performed using partial least square (PLS-SEM) method with SmartPLS 3 (<https://www.smartpls.com/>) (Hair et al., 2014). 15 questions from the survey were used to

develop the formative-formative type higher-order construct model using the embedded two-stage approach, as shown in Figure 4.3. Each item contributes to the formation of the construct, and they are not interchangeable, therefore, a formative-formative type model is used in the study. The lower-order constructs of the model are attitude (ATT), subjective norm (SN), perceived behavioral control (PBC), behavioral morality (BM), behavioral willingness (BW) and knowledge (KNO). Intention (INT) and behavior (BEH) are the general higher-order constructs. In the embedded approach, the scores of the lower-order constructs are added as variables to the higher-order constructs.

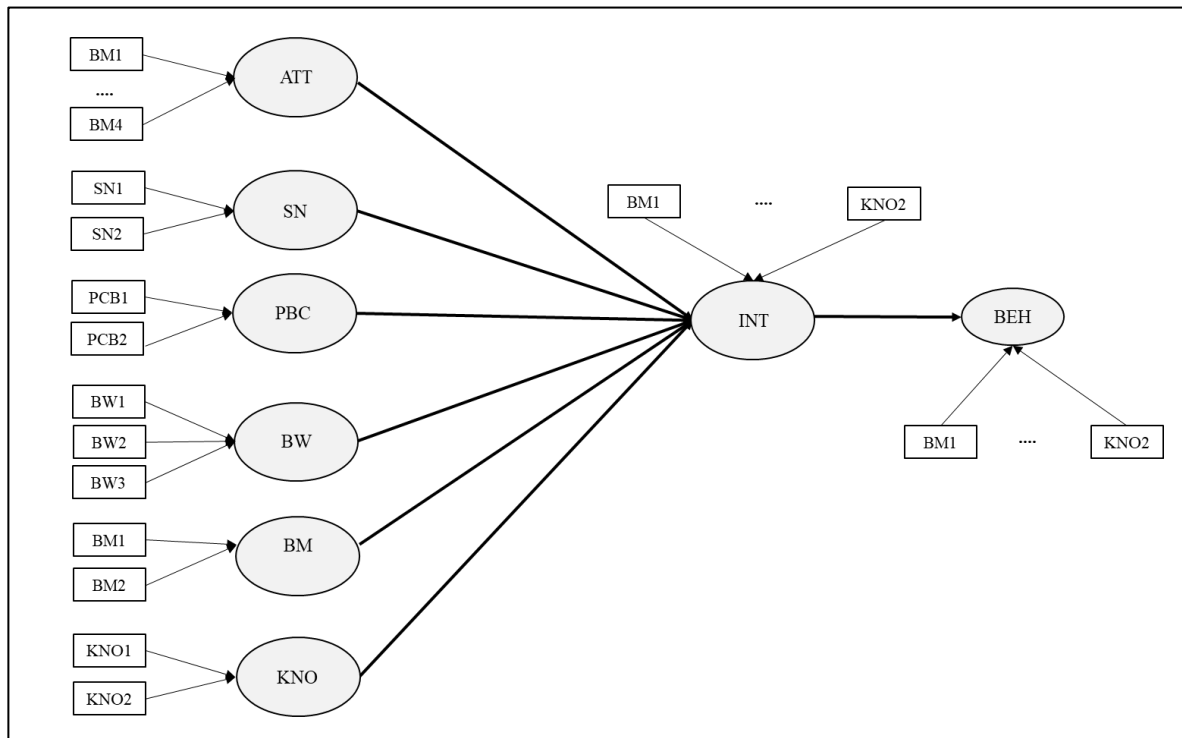


Figure 4.3 Formative-formative type model of the extended TPB (embedded two-stage approach)

To validate the formative-formative type higher-order construct, the measurement model is evaluated in a two-step procedure. In the first step, collinearity issues are checked. There are no collinearity issues with the items (questions) of lower-order constructs, as the VIF values are all lower than the conservative threshold of 3, as shown in Table 4.3.

Table 4.3 VIF, outer loading, t and p-value of constructs

| Constructs - Items | VIF | t-value | Outer loading | p-value |
|--|------------|----------------|----------------------|----------------|
| Attitude | | 7.482 | | 0 |
| I want to conserve stream for the future generation | 1.329 | 1.62 | 0.48 | |
| I will be upset if my activities harmed stream | 1.833 | 3.6 | 0.81 | |
| The stream is the lifeline of the region | 1.537 | 1.32 | 0.55 | |
| I have benefitted from VFS | 1.308 | 2.01 | 0.46 | |
| Subjective Norm | | 0.90 | | 0.367 |
| Neighbors are my close friends | 1.468 | 3.15 | (-0.45) | |
| I will implement VFS if most of my neighbors do | 1.899 | 9.91 | 0.87 | |
| Perceived Behavioral Control | | 4.26 | | 0 |
| VFS improves the aesthetics of my property | 1.71 | 1.67 | 0.79 | |
| VFS improves wildlife habitat in the region | 2.028 | 3.95 | 0.94 | |
| Knowledge | | 3.88 | | 0 |
| I have heard about VFS | 1.77 | 5.19 | 0.91 | |
| I know about stream water quality | 1.395 | 1.73 | 0.59 | |
| Behavioral Morality | | 4.84 | | 0 |
| Protecting the environment is important to me | 2.199 | 2.46 | 0.96 | |
| I have a moral obligation to maintain good water quality | 2.041 | 1.07 | 0.82 | |
| Behavioral Willingness | | 7.78 | | 0 |
| I will implement VFS if volunteers plant it | 1.592 | 3.73 | 0.75 | |
| I will implement VFS for cleaner runoff | 1.313 | 2.76 | 0.65 | |
| I will if I can plant fruit trees in VFS | 1.652 | 1.04 | 0.61 | |

In the second step, the test statistic t and its significance p of the indicator outer weights (relative) and outer loading (absolute) are evaluated by running a bootstrap of 5000 samples. Items with significant outer weight ($p < 0.1$) and/or outer loading greater than 0.5 are retained (Hair et al., 2014). These outcomes support the validity of the formative-formative type construct. The redundancy analysis to confirm convergent validity could not be performed, as global single items for the constructs were not considered in the questionnaire.

In the structural model, a conservatively significant ($p < 0.1$) path coefficient of 0.593 with a t -value of 7.95 is obtained by bootstrapping 5000 samples between INT and BEH. The predictive power of the structural model is assessed by the coefficient of determination, R_{adj}^2 that is 0.342 with a t -value of 3.649, which suggests the significant extent of the model effect. Out of sample predictive power is assessed using the blindfolding method in SmartPLS 3. Using the blindfolding method, Q^2 of 22% is recorded for both BEH and INT, which depicts medium predictive relevance of the model.

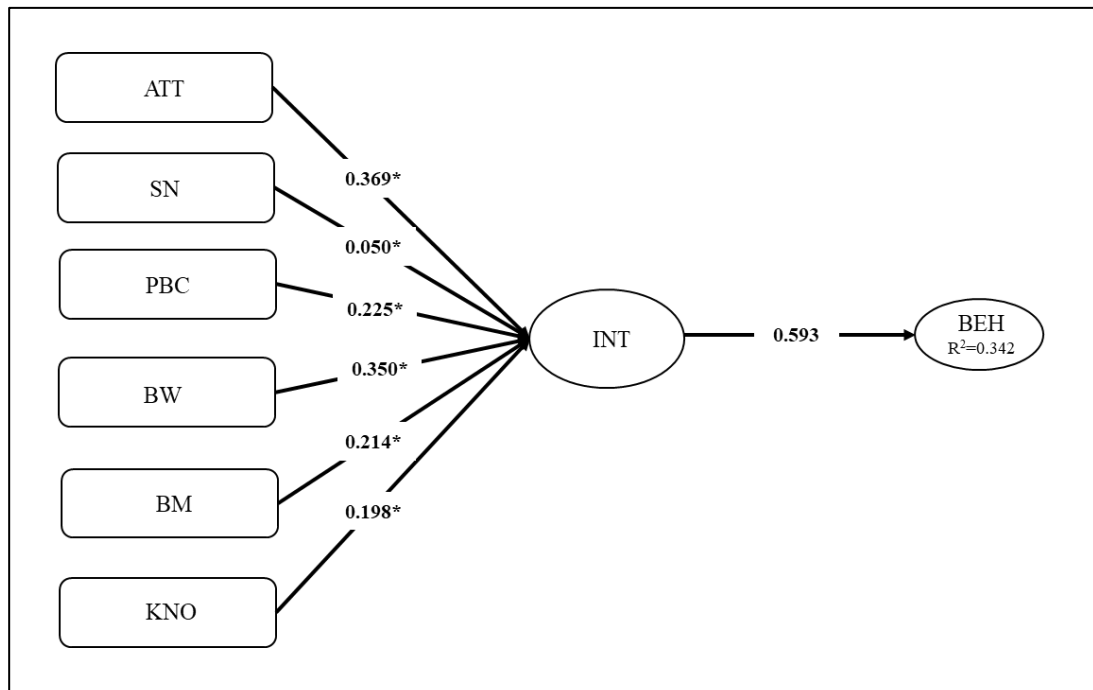


Figure 4.4 Simplified higher-order formative-formative type PLS-SEM model of extended TPB results

*Total effects of extended repeated indicator approach

As shown in Figure 4.4, the attitude of the farmers has the highest effect on whether or not they will retain or extend the width of VFS. They also perceive there exist some benefits of VFS that could improve the character of their field, which is evident by the PBC having a higher effect on intention (0.225). The farmers are not majorly influenced by the decision of their peers as it showed a non-significant effect on intention (0.05). From the extended constructs, it can be seen that farmers are more willing to have VFS on their fields if support is provided to them in the form of volunteers to help with the VFS and if farmers can yield fruits from VFS. The impression of VFS being capable of generating cleaner runoff (overland flow) from their fields also makes it agreeable for the farmers to have VFS in their fields. The moral inclination to protect the environment for future generations and to maintain good water quality is also strong amongst the farmers, as recorded by a high effect of BM on intention (0.214). Knowledge scored the least significant effect (0.198) on intention. It goes on to prove that depending on the task at hand, knowing does not always transcend into an intent to act. The loading of intention on behavior is 0.593, which identifies with the positive outlook farmers have towards VFS by the end of the survey.

4.3.2 VFSSMOD-W Modeling

Six different classes of fields are analyzed for four widths of VFS: 2, 5, 10, and 20 m. There exist natural buffers in the agricultural fields in the study area, which are not managed. This has been modeled in VFSSMOD-W as an ‘actual’ case by using alfalfa as vegetation. The effect of VFS is simulated by using tall fescue as the VFS vegetation. Two cases ‘actual’ and ‘VFS’ are simulated to help the agents decide the comparison of soil losses. Simulations are performed for all the rainfall events during the period between 1998 – 2008.

As shown in Figure 4.5, VFS of 20 m width performs consistently better compared to smaller widths. This indicates that opting for a VFS with larger width is the optimal solution to prevent soil losses in the agricultural fields. However, it should be noted that in ABM, the choice of width of VFS by agents is not solely dependent on retention efficiency.

VFSSMOD-W is used in this study as a tool to obtain the difference in soil erosion and retention by a managed VFS and natural case only. The complete removal of VFS is not foreseen, as the conversion of riparian land without VFS into managed or natural VFS is not. Such cases may be of interest in other studies with different land use characteristics. If a study is entirely

dependent on a detailed design of VFS including vegetation, more sophisticated modeling with relevant sensitivity analysis; calibration and validation are recommended to be performed.

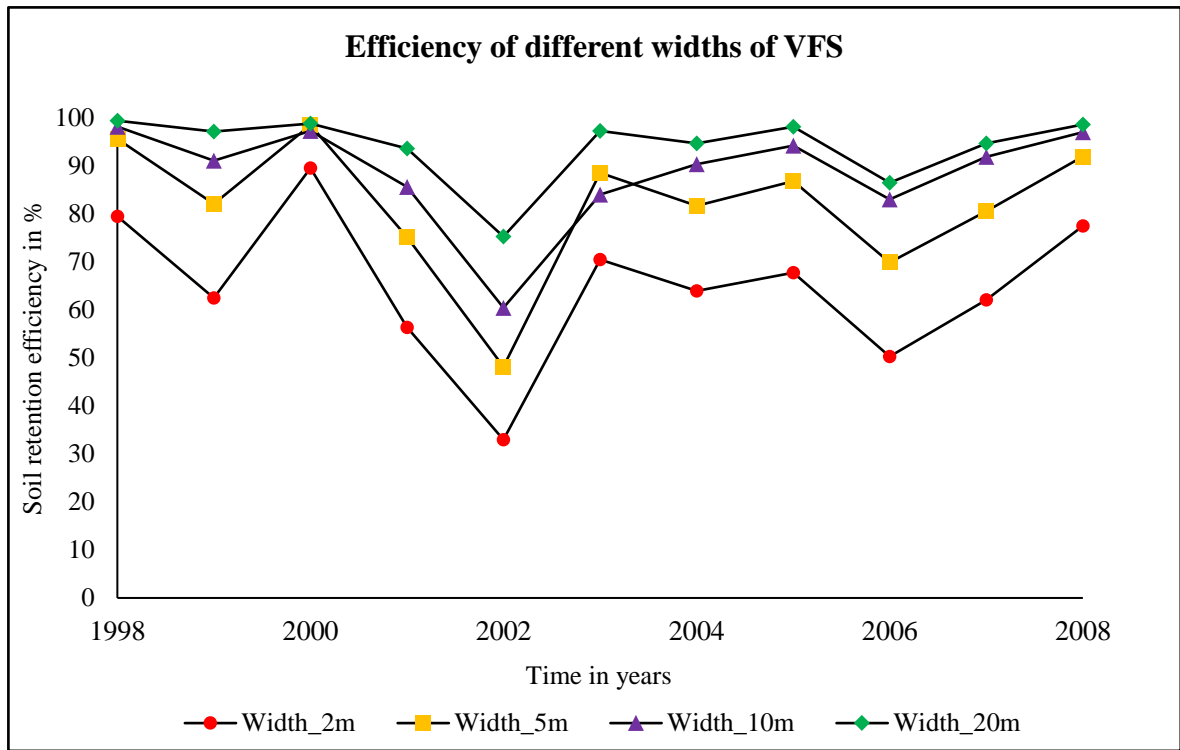


Figure 4.5 Performance efficiency of different widths of VFS in soil retention for all classes combined together

4.3.3 ABM Modeling

The agents in ABM are assigned an initial buffer width same as the actual width reported by the farmers in the survey. Though it is evident from Figure 4.5 that a larger width of VFS will reduce soil loss to a greater extent, it may not be the preferred choice of the farmers. This is because a larger width would imply loss of productive land and, subsequently, crop yield and income for the farmers. Farmers will also have to consider the annual maintenance cost that VFS would incur. Here, the behavioral classification and respective utility functions of farmers come into focus.

Based on the behavioral categorization and the utility function, the agents decide on the width of VFS once every three years, as shown in Figure 4.6. At the beginning of the simulation, 9% of the agents have a VFS width of 2 m, 37% of 5 m, 20% of 10 m and 33% of 20 m. By the

end of the simulation period, based on the utility generated over the years from the activities, 20% of agents opt to have a VFS of 2 m width, 26% of 5 m, 12% of 10 m and 42% of 20 m.

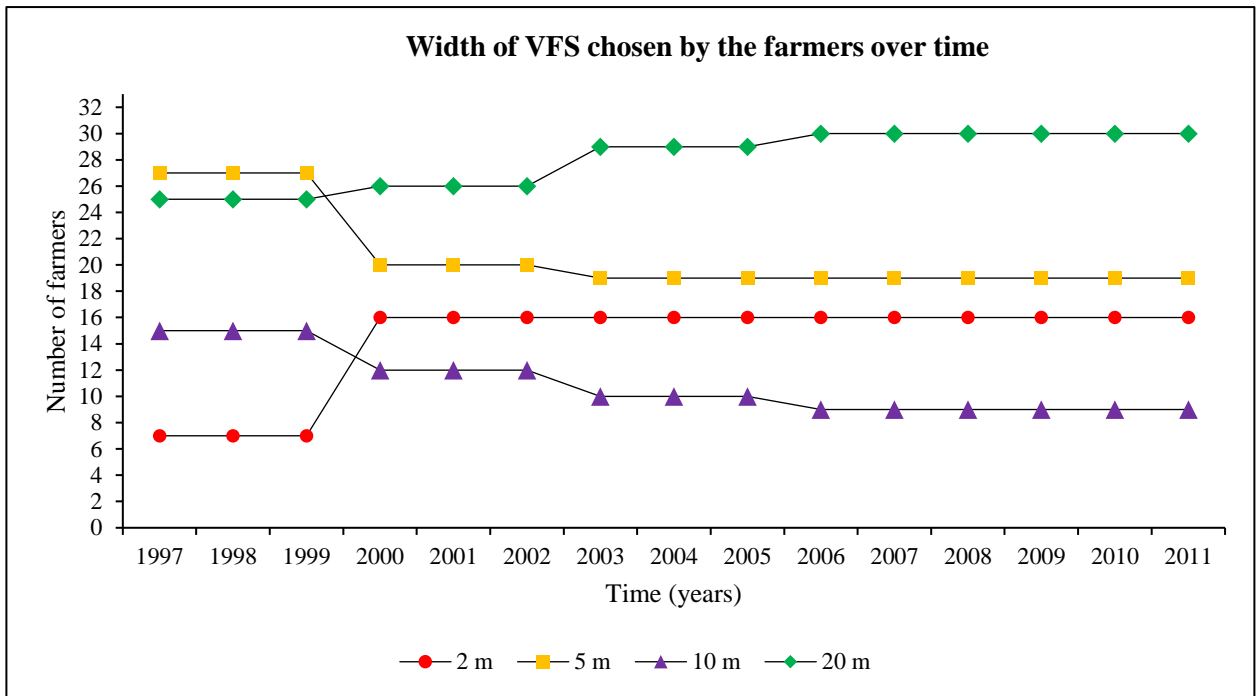


Figure 4.6 Decision of the agents on the width of VFS at the end of every three years

Depending on the willingness to manage the VFS based on the different benefits, 40 (54%) farmers expressed strong agreement, and 34 (46%) farmers showed a mild agreement to ‘don’t know’ in the onsite survey. In the developed ABM, by the end of the simulation period, 39 agents were convinced of the benefits of VFS and hence have opted for larger (10 m and 20 m) widths of VFS and those agents that showed milder agreement have chosen the smaller (2 m and 5 m) widths of VFS as seen in Table 4.4.

Table 4.4 Agent decision depending on the behavioral categorization

| Agent behavioral type | Width of VFS | 1998 | 2000 | 2003 | 2006 | 2009 |
|------------------------------|---------------------|-------------|-------------|-------------|-------------|-------------|
| Perceptive | 2 m | 0 | 0 | 0 | 0 | 0 |
| | 5 m | 1 | 0 | 0 | 0 | 0 |
| | 10 m | 1 | 1 | 0 | 0 | 0 |
| | 20 m | 2 | 3 | 4 | 4 | 4 |
| Proactive | 2 m | 1 | 11 | 11 | 11 | 11 |
| | 5 m | 5 | 0 | 0 | 0 | 0 |
| | 10 m | 1 | 0 | 0 | 0 | 0 |
| | 20 m | 4 | 0 | 0 | 0 | 0 |
| Interactive | 2 m | 5 | 5 | 5 | 5 | 5 |
| | 5 m | 19 | 19 | 19 | 19 | 19 |
| | 10 m | 9 | 9 | 9 | 9 | 9 |
| | 20 m | 16 | 16 | 16 | 16 | 16 |
| Bounded rational | 2 m | 1 | 0 | 0 | 0 | 0 |
| | 5 m | 2 | 1 | 0 | 0 | 0 |
| | 10 m | 4 | 2 | 1 | 0 | 0 |
| | 20 m | 3 | 7 | 9 | 10 | 10 |

During the survey, perceptive farmers expressed their intention to have managed VFS in their agricultural field. They understand the long-term environmental benefits of having VFS in the region and their field. This can be seen in Table 4.4, which represents the change in the agents' decisions with respect to behavioral categorization. The decision rule of perceptive agents allows them to increase the width of VFS unless they have a negative utility. It can be seen that as per their behavioral description, 2 of the perceptive agents have increased the width of VFS to 20 m by the end of the simulation period. A similar condition is observed from the bounded rational agents. These agents comprehend not only the utilities generated but also the short-term and long-term rewards of having larger widths of VFS. Since these agents perceive both monetary and environmental benefits, they gravitate towards larger widths of VFS.

We observe that the proactive agents adopt 2m as their width of VFS by the end of the simulation period. Proactive farmers would try to maximize their profit and hence adopt the minimum possible option as simulated. The lesser the width of the VFS, the more active the field for agriculture is made available, which increases their income. The decision rule for proactive agents lets them retain their initial width unless the current utility is less than the previous period's utility upon increasing the width of VFS. Being profit-oriented is the characteristic choice of proactive agents.

Proactive farmers encourage interactive farmers to decrease the width of VFS, while perceptive farmers encourage them to increase the width. Since the number of perceptive farmers in the study area is less, the proactive farmers sway the interactive farmers. However, it should be noted that interactive farmers are also subjected to the influence of bounded rational farmers. The number of bounded rational and proactive farmers is similar, thus putting the interactive farmers in a state of limbo. Therefore, in ABM, interactive agents have maintained their initial width until the end of the simulation period exhibiting no change. If bounded rational agents are well made aware of the environmental benefits of having wider VFS, they are also expected to increase the width of VFS as the combined effect of the subjective norm and morality is greater than perceived behavioral control.

The varying degrees of the area owned by the respondents, along with their behavioral alignment have led the agents to not make a definite choice of a single VFS width which can also be witnessed in the real world. It must be noted that this study is modeled for the current generation of landowners and their current land-use practices only. This cannot be transferred to their offspring or the next generation as the behavioral orientation, market, economics could be completely different.

4.4 Conclusions

The results of VFSSMOD-W show that having a managed VFS is more effective in retaining soil loss occurring in the agricultural field when compared to the natural case, which is the current situation of the farmers in the Larqui river basin, Chile. The larger width of VFS performs the best, which is evident from evaluating different VFS widths between 2 - 20m. This study revealed that the farmers in the Larqui basin are not opposed to the idea of having a VFS

as long as the utility generated stays positive. This has been proved from the developed interdisciplinary ABM and the on-site survey.

Farmer behavior whether individual or as a community, is difficult and complex to capture. Patterns from the empirical data derived from a survey are used to form explicit assumptions about the behavioral categories of the farmers and behavioral observations from the real world with the backing of the theoretical perspective of TPB. ABM corroborates the complex network of understanding farmer behavior by TPB. It provides a great insight into the policies that could be developed in the future for the farmers to motivate them to prevent soil erosion using VFS as a sustainable approach. The understanding from this study could be further used to develop policies that motivate farmers to adopt sustainable agricultural and water management practices. The developed approach of combining the observed data, theoretical behavior model and agent-based modeling coupled with an environmental model can also be extended to other socio-hydrological or socio-environmental studies for developing tailor-made management policies.

However, it should be noted that economic, political and social dynamics affects the decision-making process. Re-creating the same response from the same set of the population at a different time duration would not yield the same results due to the changes in the economy, social awareness, and personal involvement experienced by the respondents in the time between the two surveys (Öhlmer et al., 1998). In addition, human behavior is said to be non-predictable as it involves non-rational aspects as well. This makes it difficult to validate a specific ABM developed for a particular dataset with an alternative dataset. This can be partially overcome by introducing a relevant proven theoretical framework to ABM, as in this study, which will improve the foundation of an integrated, complex quantitative framework, thus can make it more robust.

Additionally, the commitment to perform the behavior would lean out with time, that is not considered in this study. If the decision is to be made within a short time duration or if the implementation in itself has a short-term existential duration, then it has better chances of being attained compared to the long-term commitment. If the time given to decide is too much, then a significant difference in the behavior can be observed. The temporal effect on the decision-making behavior of farmers can be analyzed in future studies. Anxiety to carry out a decision tendency to not follow through will also affect the implementation of a behavioral intention in

reality. This can be analyzed and reduced by the policymakers by frequently interacting with the farmers and motivating them. Results of such efforts can also be evaluated in future studies.

One of the restrictions of such studies with a limited population is a relatively low statistical robustness due to the low sample size, which was overcome by using expert-based knowledge. Low sample size can be attributed to the combined aspects of geographical limitation, farmer population who had fields adjacent to the river and were dependent on the river, the willingness of farmers to participate in a survey, limited time to name a few. Since this paper addressed socio-hydrological aspects and not pure social science, an interdisciplinary attempt was done to develop a balanced combination of social scientific and natural scientific tools for modeling human-environmental feedbacks. The case study may serve as a proof of concept but not yet a general solution. In future studies, a large sample size collection to prove the statistical stability of the theoretical model should be ensured by choosing a study area with a large sample population. Furthermore, other fields of environmental management and other socio-economic conditions could be investigated.

Acknowledgment

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5. Conclusions and Outlook

Integrated river basin management (IRBM) involves the management of the river and its basin from a cross and inter-disciplinary perspective. It aims to maximize the socio-economic aspects while maintaining/conserving/protecting the quality and biodiversity of the ecosystem. Implementation of IRBM has become crucial with decreasing water quality, declining water resources and the collapse of the balance of ecosystems worldwide. As discussed, the physical implementation of IRBM faces challenges that can be overcome by considering the river basin as a system. Under such consideration, optimization becomes a powerful tool with which multi-level, integrated aspects can be analyzed, and decisions can be made in the best interest of the river basin and its entities. An optimization model acts as an educative tool in decision-making adaptable under different conditions (Horne et al., 2016). Different variations in the application of bio-inspired optimization algorithms to optimize different aspects of IRBM are covered in this thesis. The thesis starts with a case study showcasing the ability of bio-inspired optimization algorithms to distribute mitigation measures within a basin to reduce long-term mean annual total nitrogen (TN) concentration by coupling the algorithms with the hydrological model. Furthermore, the prospect of developing an optimized tailor-made policy with stakeholder involvement is evaluated. This entails an agent-based model coupled with a vegetative filter strip model backed by a social behavioral theory.

Though extensive research on the application of bio-inspired optimization techniques on land use and urban development planning has been carried out, application in the field of optimizing river basin management plans or spatial distribution of measures is still at its nascent stage. In Chapter 3, ACO and PSO are used to optimize the distribution of mitigation measures in a river basin. The algorithms evaluate different combinations of measures for the upper Fuhse model. It emphasizes on the aspect of identifying the applicable measures to improve the water quality status in IRBM. The objective function of the algorithms was to maximize long-term annual mean TN reduction at the Peine gauging station (basin outlet) from 2006 to 2011. Measures on crop and sewage treatment plant management are considered as these are identified to be the primary sources of TN pollution in the Fuhse river. The combination of measures selected by ACO and PSO reduced the long-term annual mean TN concentration by 18.26 and 18.25 %, respectively.

By evaluating the TN concentration on river reaches at the subbasin level, it can be seen that ACO performs slightly better than PSO though overall, they are on par with each other.

It is essential to evaluate which measures or practices work best for a river basin as each has different land use patterns, hydrological processes and stakeholder practices. Only after such an evaluation can a customized river basin management plan be developed. Multiple combinations of measures could yield the reduction achieved by the algorithm selected combination. This can be contained by developing a multi-criteria optimization considering costs, benefits, nutrient management, and ecological evaluation as criteria in the algorithms. This study should be considered a ‘stepping-stone’ research to explore the abilities of bio-inspired techniques in a hydrological model coupled with the spatial distribution of mitigation measures. In this study, only a few agricultural measures on crop management and the efficiency of sewage treatment plants were considered for the spatial distribution of measures as it is the first of its kind. Future studies could include multi-objective, multi-constraint combinatorial aspects of the IRBM measures. This could include cost, benefits and social acceptance of measures (environmental and monetary), hydro-morphological measures, ecosystem services, agricultural yield etc.

The complex nature of human behavior has been of interest for many years. Many researchers have studied research on modeling and predicting human behavior from past behavior. In Chapter 5, Optimization from a planning and decision-making perspective is undertaken using theoretical social-behavioral models. In this study, data on the attitude, knowledge, subjective norm, perceived behavioral control, morality, and willingness of farmers from the Larqui river basin, Chile, is collected by performing an onsite survey. Using data from the survey, a behavioral model is developed based on the modified Theory of Planned Behavior (TPB). An agent-based model (ABM, in NetLogo) to simulate social and environmental interaction is developed by coupling it with a vegetative filter strip model (VFSSMOD-W). This framework is used to find the optimized width of VFS and the adoption of VFS to prevent soil erosion from agricultural fields by the farmers. The results showed that the farmers in the basin would adopt VFS if it prevented soil losses and their utility stayed positive. Though some farmers know the current environmental condition, further awareness could be created by involving them in farmer organizations. However, one should note that knowledge doesn’t always transcend into implementation, and some form of positive incentives should be provided to motivate farmers to adopt sustainable practices. Because

of multiple underlying circumstances, intricate and interrelated aspects, reproducing similar results from human behavior is complex. This study proves that combining meteorological, hydrological, and agricultural data with a theoretical social model and ABM could be used to develop specific plans or management policies for river basins addressing environmental issues.

Without active stakeholder involvement and cooperative working with decision-makers, as proved time and again, it would be impossible to change the water bodies' status. Eventually, plans or policies developed without stakeholders will run into the enforcement problem (Jaspers, 2003). Therefore, one of the crucial issues of IRBM is stakeholder participation. Though lessons could be learned from other river basins, the basin characteristics, key issues, and plans to overcome them are unique to each river basin and must be addressed accordingly. Interactive decision-support systems with faster converging algorithms (short computational time) that allow real-time computation of various scenarios are required. And the bountiful field of flexible, adaptable bio-inspired algorithms is the apt optimization tool for such complex applications.

However, one should remember the No Free Lunch Theorems for optimization (Wolpert and Macready, 1996). According to this theorem, there exists no one best universal algorithm that can be applied to all optimization problems. If one algorithm works better, the better-performing algorithm's accomplishment cannot be guaranteed for a completely different data set or problem. And the worse-performing algorithm could efficiently perform better for a different problem. The reason can be attributed to the fact that the inference is drawn from a sample data set, and the result is probabilistic in nature. Also, the sample dataset could differ for different problems, thus altering the performance of the algorithm. This makes the field of metaheuristic bio-inspired optimization very attractive, opens the door for the invention of new algorithms, and improves the performance of existing algorithms through modification and hybridization. The focal point of the thesis is to demonstrate the versatility and adaptability of bio-inspired optimization techniques and to inspire more researchers to gain better insight into efficient bio-inspired algorithms to solve large-scale real-world IRBM issues.

Software availability: The input data used in Chapters 3 and 4 are publicly available via the websites of the providers. Climate data were collected from the German weather service (Deutscher Wetterdienst). The national medium-scale soil map and database (BÜK 200) was published by the Federal Institute for Geosciences and Natural Resources (Bundesanstalt für Geowissenschaften und Rohstoffe). The Lower Saxony Water Management, Coastal Defense and Nature Conservation Agency (NLWKN) provided the data on streamflow, water quality, and discharge from sewage treatment plants. The HYPE model used in this study was published by Lindström et al., 2010 at <https://doi.org/10.2166/nh.2010.007>. The source code can be downloaded on the SourceForge website (<https://sourceforge.net/projects/hype/files/>). The code for the ACO and PSO optimization techniques was written in python 3.6.

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Appendix A

Supplementary materials of Chapter 2

Table. 2.I List of some of the popular bio-inspired metaheuristic algorithms

| Abbreviation | Full name | Reference | Year |
|--|---------------------------------------|----------------------------------|------|
| Swam-Intelligence based bio-inspired algorithms | | | |
| SDS | Stochastic Diffusion Search | (Bishop, 1989) | 1989 |
| ACO | Ant colony optimization | (Dorigo, 1991) | 1991 |
| PSO | Particle Swarm Optimization | (Eberhart and Kennedy, 1995) | 1995 |
| SA | Shark Algorithm | (Hersovici, et al., 1998) | 1998 |
| FSO | Fish Swarm Optimization | (Li et al., 2002) | 2002 |
| SFLA | Shuffled Frog Leaping Algorithm | (Eusuff and Lansey, 2003) | 2003 |
| SCA | Society and civilization optimization | (Ray and Liew, 2003) | 2003 |
| BH | BeeHive | (Wedde et al., 2004) | 2004 |
| ABC | Artificial Bee Colony | (Karaboga, 2005) | 2005 |
| BCO | Bee Colony Optimization | (Teodorovic and Dell’Orco, 2005) | 2005 |
| CSO | Cat Swarm Optimization | (Chu et al., 2006), | 2006 |
| HBMO | Honey Bee Mating Optimization | (Afshar et al., 2007) | 2007 |
| BEA | Bees Algorithm | (Pham et al., 2007) | 2007 |
| FBSA | Fast Bacterial Swarming Algorithm | (Chu et al., 2008) | 2008 |
| RIO | Roach Infestation Optimization | (Havens et al., 2008) | 2008 |
| BO | Bumblebees Optimization | (Comellas and Matrinez, 2009) | 2009 |
| CS | Cuckoo Search | (Yang and Deb, 2009) | 2009 |
| FA | Firefly Algorithm | (Yang, 2009) | 2009 |
| GSO | Glowworm Swarm Optimization | (Krishnanand and Ghose, 2009) | 2009 |
| LCA | League Championship Algorithm | (Kashan, 2009) | 2009 |
| BFO | Bacterial Foraging Optimization | (Passino et al., 2010) | 2010 |
| JTF | Japanese Tree Frogs | (Hernández and Blum, 2012) | 2010 |
| TCO | Termite Colony Optimization | (Hedayatzadeh et al., 2010) | 2010 |
| ASO | Anarchic Society Algorithm | (Ahmadi-Javid, 2011) | 2011 |

| | | | |
|------|--------------------------------------|--------------------------------|------|
| BSO | Brain Storm Optimization | (Shi, 2011) | 2011 |
| TLBO | Teaching Learning Based Optimization | (Rao et al., 2011) | 2011 |
| BA | Bat Algorithm | (Yang and Gandomi, 2012) | 2012 |
| GSR | Great Salmon Run | (Mozaffari et al., 2012) | 2012 |
| KH | Krill Herd | (Gandomi and Alavi, 2012) | 2012 |
| DSO | Dolphin Swarm Optimization | (Wu et al., 2016) | 2013 |
| SSO | Social Spider Optimization | (Cuevas et al., 2013) | 2013 |
| CRO | Coral Reefs Optimization | (Salcedo-Sanz et al., 2014) | 2014 |
| CFA | Cuttle Fish Optimization | (Eesa et al., 2014) | 2014 |
| GWO | Grey Wolf Optimizer | (Mirjalili et al., 2014) | 2014 |
| SOS | Symbiotic Organisms Search | (Cheng and Prayogo, 2014) | 2014 |
| SMO | Spider Monkey Optimization | (Bansal et al., 2014) | 2014 |
| CSO | Chicken-Swarm Optimization | (Meng et al., 2014) | 2014 |
| JA | Jaguar Algorithm | (Chen et al., 2015) | 2015 |
| ALO | Ant Lion Optimizer | (Mirjalili, 2015b) | 2015 |
| MBO | Monarch Butterfly Optimization | (Wang et al., 2015) | 2015 |
| MFOA | Moth-flame optimization algorithm | (Mirjalili, 2015a) | 2015 |
| PPA | Prey-Predator Algorithm | (Tilahun and Ong, 2015) | 2015 |
| ABO | African-Buffalo Optimization | (Odili et al., 2015) | 2015 |
| EHA | Elephant Herding Algorithm | (Wang et al., 2015) | 2015 |
| PIO | Pigeon-Inspired Optimization | (Duan and Qiao, 2014) | 2015 |
| SSA | Social Spider Algorithm | (James and Li, 2015) | 2015 |
| DA | Dragonfly algorithm | (Mirjalili, 2016) | 2016 |
| SWA | Sperm Whale Algorithm | (Ebrahimi and Khomehchi, 2016) | 2016 |
| WOA | Whale Optimization Algorithm | (Mirjalili and Lewis, 2016) | 2016 |
| MFO | Mosquito Flying Optimization | (Alauddin, 2016) | 2016 |
| CA | Camel Travelling Behavior | (Ibrahim and Ali, 2016) | 2016 |
| BSA | Bird-Swarm Algorithm | (Meng et al., 2016) | 2016 |
| CSA | Crow Search Algorithm | (Askarzadeh, 2016) | 2016 |

| | | | |
|------|---|--------------------------------------|------|
| RDA | Red Deer Algorithm | (Fard and Hajiaghaei-Keshteli, 2016) | 2016 |
| GOA | Grasshopper Optimisation Algorithm | (Saremi et al., 2017) | 2017 |
| KA | Kidney Algorithm | (Jaddi et al., 2017) | 2017 |
| KWA | Killer Whale Algorithm | (Biyanto et al., 2017) | 2017 |
| WSA | Salp Swarm Optimization | (Mirjalili et al., 2017) | 2017 |
| MRA | Mushroom Reproduction Optimization | (Bidar et al., 2018) | 2018 |
| MIA | Meerkats Inspired Algorithm | (Al-Obaidi et al., 2018) | 2018 |
| CBA | Cheetah Chase Algorithm | (Goudhaman, 2018) | 2018 |
| HHO | Harris Hawks optimization | (Bairathi and Gopalani, 2020) | 2019 |
| SO | Sailfish Optimizer | (Shadravan et al., 2019) | 2019 |
| SSA* | Squirrel Search Algorithm | (Jain et al., 2019) | 2019 |
| EPC | Emperor-Penguins Colony | (Harifi et al., 2019) | 2019 |
| BWOA | Black Widow Optimization Algorithm | (Hayyolalam and Kazem, 2020) | 2020 |
| ChoA | Chimp Optimization Algorithm | (Khishe and Mosavi, 2020) | 2020 |
| COA | Coronavirus Optimization Algorithm | (Martínez-Álvarez et al., 2020) | 2020 |
| MOA | Mayfly Optimization Algorithm | (Zervoudakis and Tsafarakis, 2020) | 2020 |
| WSA | Water Strider Algorithm | (Kaveh and Dadras Eslamlou, 2020) | 2020 |
| HHOA | Horse Herd Optimization Algorithm | (MiarNaeimi et al., 2021) | 2021 |
| ACVO | Anti-Coronavirus Optimization Algorithm | (Emami, 2022) | 2022 |

Non-Swam-Intelligence based bio-inspired algorithms

| | | | |
|---------|-----------------------------|-------------------------|------|
| GA | Genetic Algorithms | (Holland, 1975) | 1975 |
| GP | Genetic Programming | (Fogel et al., 1966) | 1992 |
| DE | Differential Evolution | (Storn and Price, 1996) | 1996 |
| GE | Gene Expression | (Ferreira, 2001) | 2001 |
| NSGA-II | Non-dominated Sorting GA-II | (Deb et al., 2002) | 2002 |

| | | | |
|------|---|------------------------------------|------|
| QBE | Queen-Bee Evolution | (Jung, 2003) | 2003 |
| WO | Weed Optimization Algorithm | (Mehrabian and Lucas, 2006) | 2006 |
| IWO | Invasive Weed Optimization | (Karimkashi and Kishk, 2010) | 2006 |
| DEMC | Differential Evolution Markov Chain | (Braak, 2006) | 2006 |
| ICA | Imperialistic Competitive Algorithm | (Atashpaz-Gargari and Lucas, 2007) | 2007 |
| MSA | Monkey Search Algorithm | (Mucherino and Seref, 2007) | 2007 |
| HIA | Human Inspired Algorithm | (Zhang et al., 2009b) | 2009 |
| ECO | Eco-inspired evolutionary Algorithm | (Parpinelli and Lopes, 2011) | 2011 |
| FPA | Flower Pollination Algorithm | (Yang, 2012) | 2012 |
| OB | Opt Bees | (Maia et al., 2013) | 2012 |
| EVOA | Egyptian Vulture Optimization Algorithm | (Sur et al., 2013) | 2013 |
| DEO | Dolphin Echolocation Optimization | (Kaveh and Farhoudi, 2013) | 2013 |

Appendix B

Supplementary materials of Chapter 3

Table 3.I Percentage long-term annual mean TN reduction at subbasin level

| Subbasin No. | % TN Reduction by ACO | % TN Reduction by PSO | Binary Difference Indicator |
|-------------------------|----------------------------------|----------------------------------|--|
| 1 | 18.27 | 18.25 | 1 |
| 2 | 0.03 | 0.03 | 0 |
| 3 | 16.33 | 16.32 | 1 |
| 4 | 0.08 | 0.08 | 1 |
| 5 | 0.0 | 0.00 | 0 |
| 6 | 7.4 | 6.58 | 1 |
| 7 | 21.79 | 21.77 | 1 |
| 8 | 0.20 | 0.20 | 0 |
| 9 | 26.78 | 26.76 | 1 |
| 10 | 6.15 | 5.43 | 1 |
| 11 | 28.33 | 28.32 | 1 |
| 12 | 6.11 | 5.41 | 1 |
| 13 | 24.71 | 24.71 | 0 |
| 14 | 33.33 | 33.33 | 0 |
| 15 | 43.86 | 43.86 | 0 |
| 16 | 0.05 | 0.05 | 0 |
| 17 | 0.0 | 0.0 | 0 |
| 18 | 0.04 | 0.04 | 0 |
| 19 | 0.0 | 0.0 | 0 |
| 20 | 0.0 | 0.0 | 0 |
| 21 | 0.0 | 0.0 | 0 |
| 22 | 0.05 | 0.05 | 0 |
| 23 | 0.10 | 0.10 | 0 |
| 24 | 0.17 | 0.17 | 0 |
| 25 | 0.00 | 0.00 | 0 |

The binary difference indicator is provided in the last column. A value of 1 indicates the subbasin reaches where ACO performs slightly better than PSO. A value of 0 indicates same performance by both algorithms.

Appendix C

Supplementary materials of Chapter 4

4.A. Figures

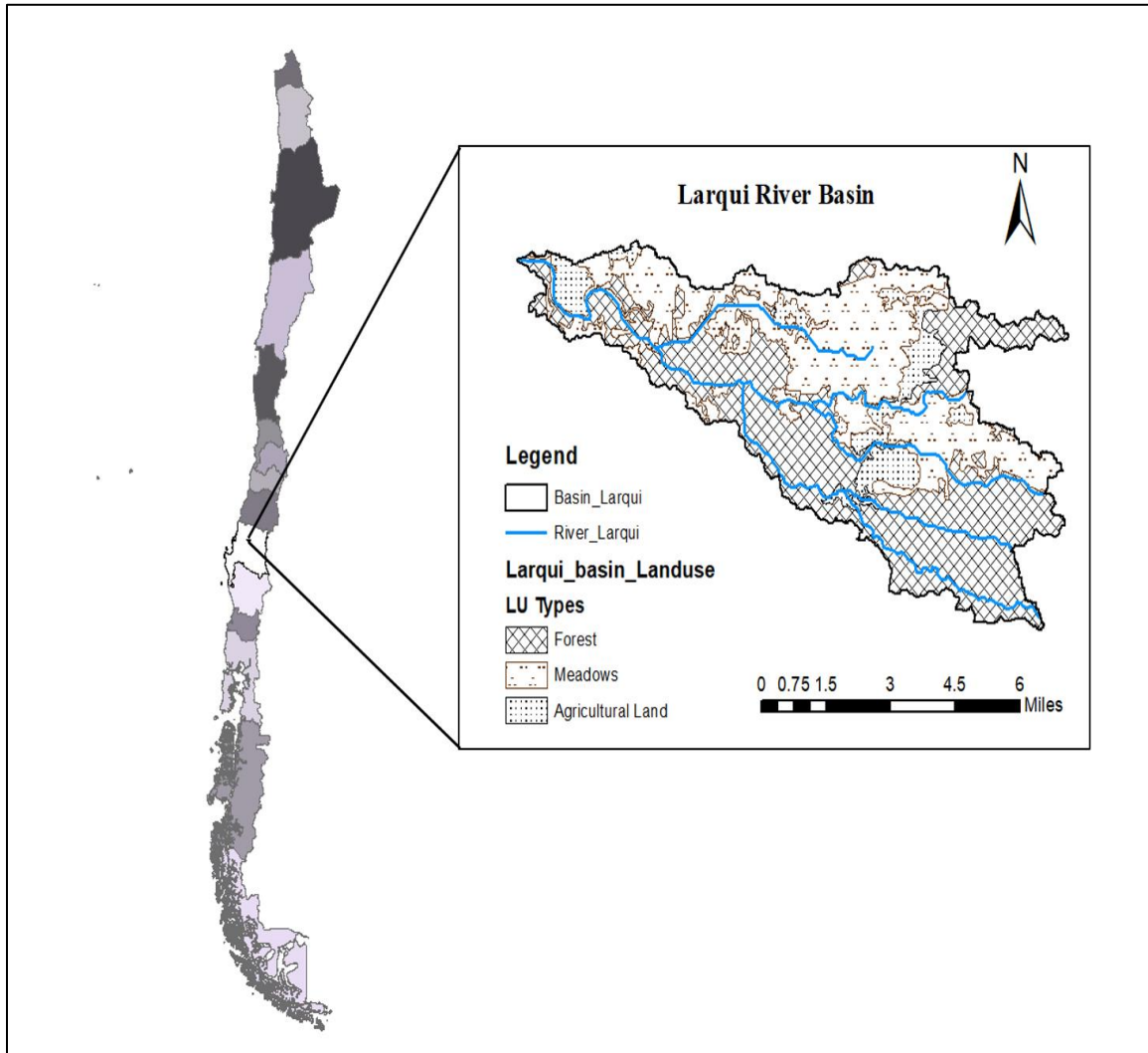


Figure 4.I Study area - Larqui river basin

Data source: DIVA-GIS (<https://www.diva-gis.org/gdata>) and Ide-Minagri (<http://ide.minagri.gob.cl/geoweb/index.php/descargas>)

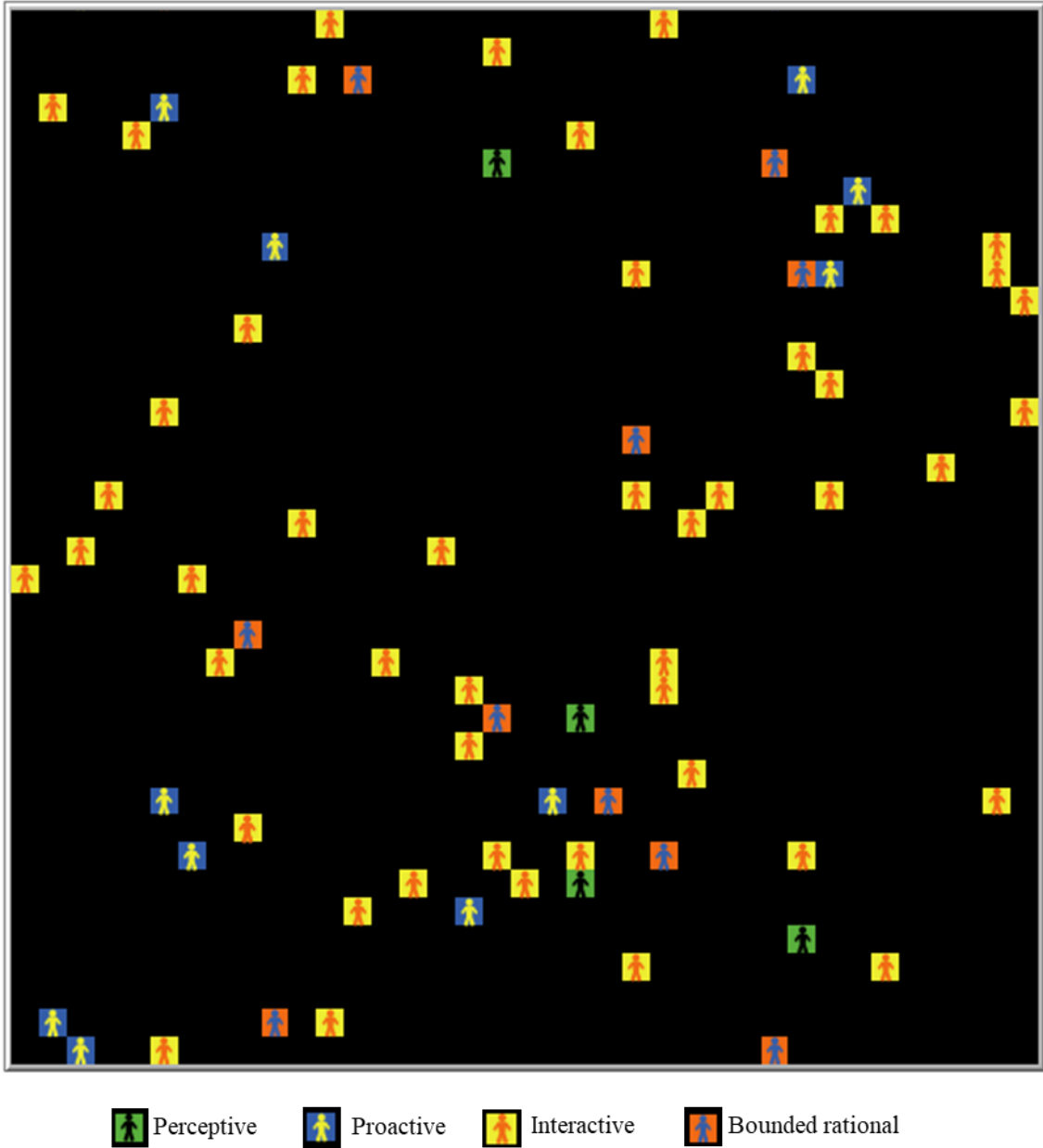


Figure 4.II Representation of the four types of agents in NetLogo

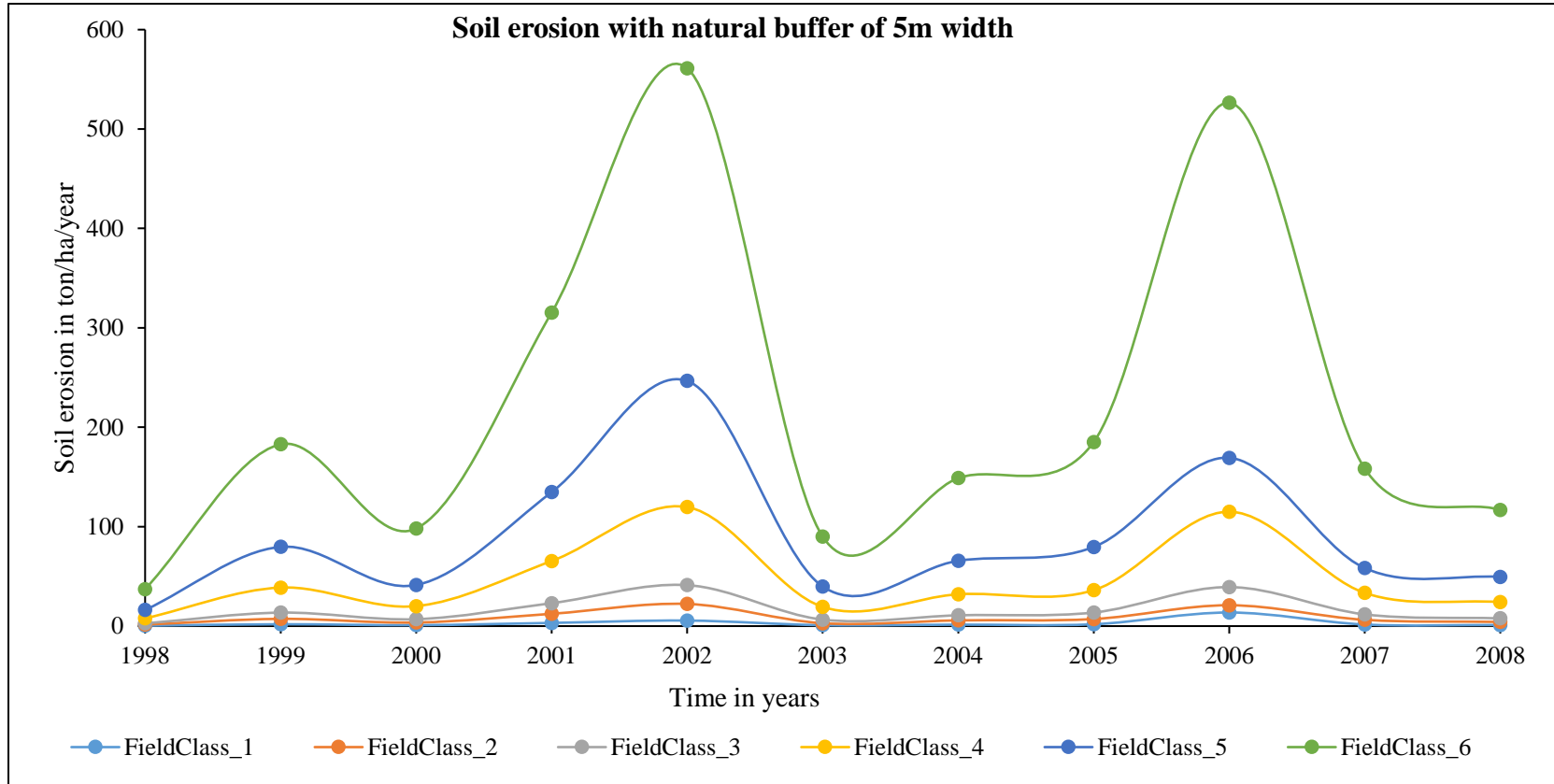


Figure 4.III Soil erosion in different field classes

Figure 4.III represents the soil losses experienced by the farmers during the simulation period for the ‘actual’ case with a 5m width buffer, which is used by most of the farmers (27 out of 74) in the study area.

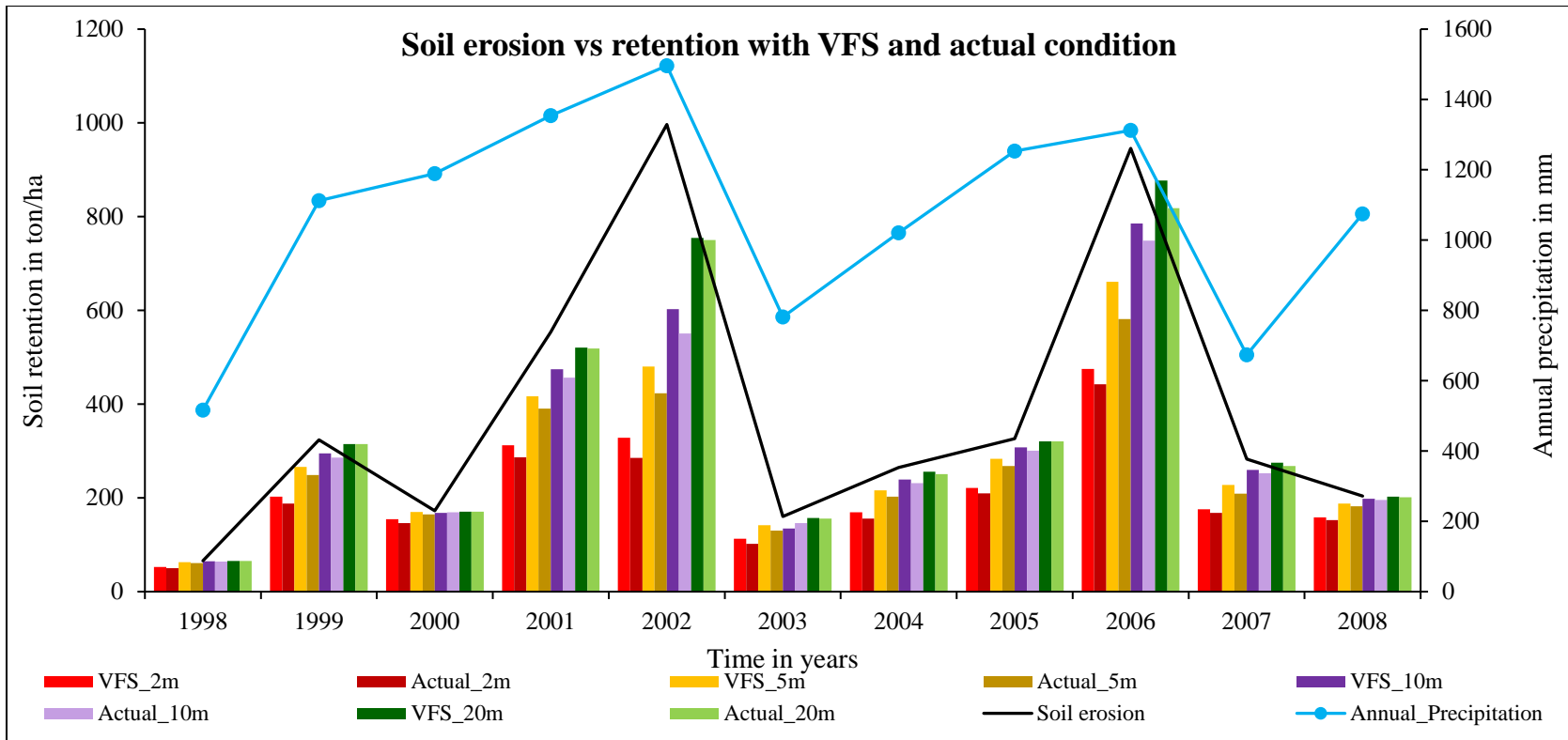


Figure 4.IV Soil erosion vs. retention with and without VFS

While the soil retention of different widths of buffer in both cases appear similar, a clear difference is observed in the years 2002 and 2006 where annual soil eroded is greater due to intensive rainfall. It can be seen that VFS performs better compared to the 'actual' case in retaining the soil losses due to erosion. Amongst the different widths of VFS, larger widths of VFS perform much better.

4.B. Tables

Table 4.I Field classes and their characteristics

| Field Class | Min. Farm Size [ha] | Max. Farm Size [ha] | Number of farmers | Swidth [m] | Slength [m] |
|--------------------|----------------------------|----------------------------|--------------------------|-------------------|--------------------|
| 1 | 0.5 | 1 | 11 | 110 | 1 Swidth |
| 2 | 2 | 5 | 31 | 153 | 1.5 Swidth |
| 3 | 5 | 10 | 13 | 170 | 0.43 Swidth |
| 4 | 11 | 29 | 8 | 311.4 | 0.54 Swidth |
| 5 | 30 | 60 | 5 | 346.5 | 0.33 Swidth |
| 6 | 61 | 200 | 6 | 447.2 | 0.25 Swidth |

Table 4.II ODD+D protocol for the developed ABM of farmer decision-making (according to the protocol developed by Müller et al. (2013))

| Outline | | Guiding questions | ODD+D Model description for the developed ABM |
|----------|--|---|---|
| Overview | I.i Purpose | I.i.a What is the purpose of the study? | <p>The purpose of the study is to develop a socio-hydrological framework to improve the acceptance of environmental measures by stakeholders. This is tested for use of vegetative filter strip as a land use management strategy to reduce soil erosion in the agricultural fields of farmers and thus prevent water pollution in the adjacent streams.</p> <p>An ABM is developed on the social theory of behavior (Theory of Planned Behavior aka TPB), and coupled with the environmental process model to model soil loss (VFSSMOD-W).</p> <p>This framework provides the perspective of farmers to the policymakers so that they can develop policies to promote the use of VFS based on the field situation.</p> |
| | | I.i.b For whom is the model designed? | Scientists, decision-makers, farmer organizations and farmers (stakeholders) |
| | I.ii Entities, state variables, and scales | I.ii.a What kinds of entities are in the model? | <p>Agents: Framers;</p> <p>Spatial units: Grids representing individual agricultural fields</p> <p>Institution: Farmer organizations;</p> <p>Environment and collectives: Larqui river basin of 74 farmers that are classified to 4 behavioral categories</p> |

| | | |
|---------------------------------------|---|--|
| | | (perceptive, proactive, interactive and bounded rational based on quantitative ordinals derived from the field survey) and 6 field class depending on the size of the agricultural field (see Table 4.1). |
| | I.ii.b By what attributes (i.e. state variables and parameters) are these entities characterized? | Agents: an agent represents one individual farmer who is the owner of the land. Spatial units: one grid represents one piece of land owned by a farmer Collectives: decision-making by the agents depending on their behavioral categorization; farmer organization. |
| | I.ii.c What are the exogenous factors/drivers of the model? | Loss of soil due to erosion in the agricultural fields, the monetary investment and benefits of VFS and the behavioral categorization of the agents |
| | I.ii.d If applicable, how is space included in the model? | Not included |
| | I.ii.e What are the temporal and spatial resolutions and extents of the model? | One-time step represents one day and the simulation was run for 10 years from 1998 to 2008. Each grid cell represents the agricultural field owned by the agent. No spatial definition is given. |
| I.iii Process overview and scheduling | I.iii.a What entity does what, and in what order? | The agents, every three years, decide if they want to expand the width of the VFS they have based on their behavioral |

| | | | |
|-----------------|---|--|--|
| | | | categorization and the utility they made over the past three years. |
| Design Concepts | II.i Theoretical and Empirical Background | II.i.a Which general concepts, theories or hypotheses are underlying the model's design at the system level or the level(s) of the submodel(s) (apart from the decision model)? What is the link to the complexity and the purpose of the model? | Based on the Theory of Planned Behavior (TPB), standardized regression weights are derived from the data collected in the survey. These weights are used in the ABM model to weigh upon the decision making of the agent. Apart from the TPB, utility function is developed that encompasses monetary values from different agricultural activities including implementation of VFS and losses due to soil loss, and benefits of implementing VFS. The results from VFSSMOD-W is the third sub-model used in this study, which provides the trigger to the agents to decide on the width of VFS based on the threshold of soil loss. |
| | | II.i.b On what assumptions is/are the agents' decision model(s) based? | The agents follow a bounded rational decision or profit-maximizing decision by considering the environmental information. Their decision is based on the decision-making rule developed for the study based on the interactions had with the farmers on-site. The rules are presented in Table .2. |
| | | II.i.c Why is a/are certain decision model(s) chosen? | The decision model used in the study is derived from the data gathered from the on-site survey and farmer interaction. |

| | | | |
|----------------------------------|--|--|---|
| | | II.i.d If the model / a sub-model (e.g. the decision model) is based on empirical data, where does the data come from? | The data is collected from the on-site survey. |
| | | II.i.e At which level of aggregation were the data available? | Individual-level |
| II.ii Individual Decision Making | | II.ii.a What are the subjects and objects of decision-making? On which level of aggregation is decision-making modeled? Are multiple levels of decision making included? | Individual agents are the subjects of decision-making while the width of the VFS is the object. Multiple levels of decision-making are not included. |
| | | II.ii.b What is the basic rationality behind agents' decision-making in the model? Do agents pursue an explicit objective or have other success criteria? | In this study, the rationality for decision making varies between different behavioral categorization. Utility maximization is considered for proactive agents. In the case of the perceptive agents' utility non-negativity is taken into account. Bounded rational and interactive agents ensure that the utility doesn't decrease. |
| | | II.ii.c How do agents make their decisions? | The agents decide based on utility function and behavioral categorization ensuring non-negative monetary values. |

| | | |
|-----------------|---|---|
| | <p>II.ii.d Do the agents adapt their behavior to changing endogenous and exogenous state variables? And if yes, how?</p> | No |
| | <p>II.ii.e Do social norms or cultural values play a role in the decision-making process?</p> | The societal influence which is defined as the subjective norm in TPB plays a role in the model. |
| | <p>II.ii.f Do spatial aspects play a role in the decision process?</p> | Yes, the fields of the agents are divided into 6 different classes for ease of calculation. However, they hardly influence decision-making. On the other hand, the width of VFS which is also a spatial entity for a field influences the soil loss, benefits gained. |
| | <p>II.ii.g Do temporal aspects play a role in the decision process?</p> | Yes. The decision of the farmer about the width of VFS is made once every three years. |
| | <p>II.ii.h To which extent and how is uncertainty included in the agents' decision rules?</p> | It is not included. |
| II.iii Learning | <p>II.iii.a Is individual learning included in the decision process? How do individuals change their decision rules over time as a consequence of their experience?</p> | Yes, individual learning is included in the model. The farmers compare the utility generated over the past three years with the current utility and change their decision accordingly. |

| | | | |
|--------------------------------|--|---|---|
| | | II.iii.b Is collective learning implemented in the model? | No, collective learning is not included in this model. |
| II.iv Individual Sensing | | II.iv.a What endogenous and exogenous state variables are individuals assumed to sense and consider in their decisions? Is the sensing process erroneous? | Sensing process is not included. |
| | | II.iv.b What state variables of which other individuals can an individual perceive? Is the sensing process erroneous? | Though no sensing process is included, the behavior of other agents influence interactive and bounded rational agents on their decision making. |
| | | II.iv.c What is the spatial scale of sensing? | No spatial scale is used. |
| | | II.iv.d Are the mechanisms by which agents obtain information modeled explicitly, or are individuals simply assumed to know these variables? | They are modeled explicitly based on the information collected from the onsite survey. |
| | | II.iv.e Are costs for cognition and costs for gathering information included in the model? | No, the cost of gathering information is not included. |

| | | |
|----------------------------|---|--|
| II.v Individual Prediction | II.v.a Which data uses the agent to predict future conditions? | Future prediction is not used in the study, however, learning from the past is used to decide for the current time-step. |
| | II.v.b What internal models are agents assumed to use to estimate future conditions or consequences of their decisions? | Not applicable |
| | II.v.c Might agents be erroneous in the prediction process, and how is it implemented? | Not applicable |
| II.vi Interaction | II.vi.a Are interactions among agents and entities assumed as direct or indirect? | Agents belonging to the bounded rational and interactive categorization interact with other agents. |
| | II.vi.b On what do the interactions depend? | The interactions depend on the behavioral categorization of the agents. |
| | II.vi.c If the interactions involve communication, how are such communications represented? | The standardized regression weight of subjective norm is used to weigh in on the behavioral entity of the agents to indicate the influence of interaction. |
| | II.vi.d If a coordination network exists, how does it affect the agent behavior? Is the structure of the network imposed or emergent? | A coordination network is not used in this study. |

| | | |
|--------------------------|--|---|
| II.vii Collectives | II.vii.a Do the individuals form or belong to aggregations that affect, and are affected by, the individuals? Are these aggregations imposed by the modeler or do they emerge during the simulation? | Yes, the farmer organization has its weight which is triggered when at least 50% of the agents join the organization. This is because such organizations partake only if at least 50% of the farmers register themselves with the organization. These are imposed depending on the information collected during the on-site survey. |
| | II.vii.b How are collectives represented? | They are represented separately as agents who interact with farmer organizations. |
| II.viii Heterogeneity | II.viii.a Are the agents heterogeneous? If yes, which state variables and/or processes differ between the agents? | The agents are heterogeneous because they represent farmers who exhibit heterogeneous behavior. The exchange will affect the results of the simulation, but the overall trend might not be affected. |
| | II.viii.b Are the agents heterogeneous in their decision-making? If yes, which decision models or decision objects differ between the agents? | The agents are heterogeneous in decision-making as defined by the decision-making rules. The object of utility function maximization, maintenance and non-negation vary depending on the behavioral categorization of the agents. |
| II.ix Stochasticity | II.ix.a What processes (including initialization) are modeled by assuming they are random or partly random? | None. |

| | | | |
|---------|-----------------------------------|--|---|
| Details | II.x Observation | II.x.a What data are collected from the ABM for testing, understanding, and analyzing it, and how and when are they collected? | The data on the number of farmers choosing different widths of VFS at every three-year interval is collect based on behavioral categorization and field classes for understanding the decision-making and analyzing it. |
| | | II.x.b What key results, outputs or characteristics of the model are emerging from the individuals? (Emergence) | The results are discussed in detail in section 3.3 |
| | II.i Implementation Details | III.i.a How has the model been implemented? | The model is developed in NetLogo. It has a simulation runtime of approx. 3 minutes when running on normal speed and the development of it took up to 6 months. |
| | | III.i.b Is the model accessible and if so where? | The model code will be provided upon request. |
| | III.ii Initialization | III.ii.a What is the initial state of the model world, i.e. at time t=0 of a simulation run? | At t=0, there are 4 perceptive agents, 10 proactive agents, 49 interactive agents, and 11 bounded rational agents. Each agent has an initial length of VFS and field class assigned based on data collected during the onsite survey. |
| | | III.ii.b Is initialization always the same, or is it allowed to vary among simulations? | Yes, it is always the same as it is the field data. |

| | | | |
|--|--------------------|---|---|
| | | III.ii.c Are the initial values chosen arbitrarily or based on data? | The initial values are based on data collection. |
| | III.iii Input Data | III.iii.a Does the model use input from external sources such as data files or other models to represent processes that change over time? | Yes, the parameters used in the model are derived from external sources. The model uses soil retention and soil loss results from VFSMOD-W and observed rainfall events. |
| | III.iv Submodels | III.iv.a What, in detail, are the sub-models that represent the processes listed in ‘Process overview and scheduling’? | The behavior equation as per TPB and utility function equation described in the paper are used. |
| | | III.iv.b What are the model parameters, their dimensions, and reference values? | Please refer to Table 4.1 for parameters of the utility function. Equations 4.1-4.5 show the utility function used in the model, and Table 4.4 depicts the standardized regression weights of behavioral function derived from the onsite survey. |
| | | III.iv.c How were sub-models designed or chosen, and how were they parameterized and then tested? | The behavioral sub-model is designed from the information collected during the on-site survey. The data fit of the TPB model is tested for reliability (Cronbach’s alpha). The parameters of the utility function sub-model are collected from the literature review. |

4.C. QUESTIONNAIRE

(1) Basic details

Name: _____

Age: _____ years

Contact information: _____

a. What is the size of your land?

_____ hectares

b. What is the length of the stream next to or through the land parcel?

_____ meters

c. There is water in the stream

1 : 2 : 3 : 4 : 5
always seasonal most days few days never

d. What crop do you grow in the land?

e. I use the stream water for irrigating my land

1 : 2 : 3 : 4 : 5
always seasonally only when required also use other source never

f. If for the question (e.) is 'also other sources' and 'never' what is the other source of water you use?

g. The irrigation system I use is

(Example: drip irrigation, central pivot, sprinkler, gravitational furrow)

h. In the future, I would like to implement another irrigation system

() Yes () No

If yes, the new irrigation system: _____

i. Please provide a rough sketch indicating the farmland, buffer strip, stream and the road to the farm

(2) Environmental knowledge

a. How is the water quality of the stream?

| | | | | | | | | |
|----------------|---|------|---|------------|---|-----|---|---------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Extremely good | | good | | don't know | | bad | | extremely bad |

b. I am concerned with the quality of water I receive

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

c. I am concerned with the quality of water in the stream

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

d. I am concerned with the quality of water in the region

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

e. I have a moral obligation to maintain water quality

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

f. How knowledgeable do you feel about water quality in your stream?

| | | | | | | | | |
|----------------|---|------|---|------------|---|-----|---|---------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Extremely good | | good | | don't know | | bad | | extremely bad |

g. Protecting the environment is important to me

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

h. The stream is the lifeline of the region

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

i. I would be upset if my activities harmed the stream

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

j. I want to conserve the stream for my future generations

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

k. I use nutrients to increase my agricultural yield

| | | | | | | | | |
|--------|---|------------|---|------------|---|---------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| always | | most times | | moderately | | organic | | never |

l. I have soil erosion from my farmland

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

m. I replace the eroded soil

| | | | | | | | | |
|--------------|---|-------------|---|--------------------|---|--------------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| every season | | once a year | | no particular time | | only when required | | never |

n. I lose nutrients excessively with the eroded soil

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

(3) Knowledge on buffer strips

a. I have heard of buffer strips before

Yes No

b. I have buffer strip in my farmland

Yes No only in some places

Reason: _____

c. The width of the buffer strip is _____ meters

d. The buffer strip I have is

() Natural (forest)

() Manmade (modified)

e. I have the buffer strip because:

f. If the answer to (b) is no then, I would like to have buffer strip in my land

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

g. Having a buffer strip has benefited me

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

h. List few uses of buffer strips

i. My neighbour has buffer strip in his/her land

() Yes

() No

j. I interact with my neighbours

| | | | | | | | | |
|-------|---|--------|---|--------------|---|-----------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| daily | | weekly | | once a month | | once in a while | | never |

k. Number of neighbours that are my close friends

| | | | | | | | | |
|------------|---|----------------|---|------|---|----------|---|------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| almost all | | more than half | | half | | very few | | zero |

l. I think the effect of buffer strips includes improved:

i. Water quality downstream

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

ii. Water quality in my stream

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

iii. Water quality in the Biobio region

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

iv. Character of my property (aesthetics)

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

v. Fish habitat

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

vi. Wildlife habitat in the region

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

vii. Flood protection downstream

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

viii. Property values will increase

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

ix. Access to buffer program payments

| | | | | | | | | |
|----------------|---|-------|---|------------|---|----------|---|-------------------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| strongly agree | | agree | | don't know | | disagree | | strongly disagree |

m. Are you a member of 'Junta de Vigilancia' or any local committee?

() Yes

() No

Local committee: _____

n. If yes, do you consult with the committee for any environmental decision making to your farm?

Yes No

Recent decision: _____

o. Has any committee or anyone has spoken to you about buffer strips in the past?

Yes No

Who?: _____

(4) Willingness to implement buffer

Would you be more willing if :

a. A buffer reduced streambank erosion

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| Yes, very willing | | willing | | may be | | not really | | never |

b. You had a say in designing your buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| Yes, very willing | | willing | | may be | | not really | | never |

c. Weeds were removed for you

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| Yes, very willing | | willing | | may be | | not really | | never |

d. A buffer made water runoff from your property cleaner

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| Yes, very willing | | willing | | may be | | not really | | never |

e. The trees and shrubs for the buffer were free

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| <hr/> | | | | | | | | |
| Yes, very willing | | willing | | may be | | not really | | never |

f. The trees were fruit or nut trees

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

g. I am allowed to sell the produce from the buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

h. You received yearly payments for your buffer costs

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

i. Volunteers planted the buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

j. You received a one-time payment for your buffer installation

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

k. You were given guidance on how to build a buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

l. Most of your neighbors installed stream buffers

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

m. Someone in your neighborhood installed a buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

n. A good friend installed a buffer

| | | | | | | | | |
|-------------------|---|---------|---|--------|---|------------|---|-------|
| 1 | : | 2 | : | 3 | : | 4 | : | 5 |
| Yes, very willing | | willing | | may be | | not really | | never |

(5) I do not want buffer strips because:

a) Takes away too much land

1 : 2 : 3 : 4 : 5
strongly agree agree don't know disagree strongly disagree

b) Doesn't make sense to have for the size of my land

1 : 2 : 3 : 4 : 5
strongly agree agree don't know disagree strongly disagree

c) Maintenance takes time and money

1 : 2 : 3 : 4 : 5
strongly agree agree don't know disagree strongly disagree

d) Would bother my neighbors

1 : 2 : 3 : 4 : 5
strongly agree agree don't know disagree strongly disagree

e) List any other obstacles you face to implement buffer strips

f) I don't want others to decide what is on my property

1 : 2 : 3 : 4 : 5
strongly agree agree don't know disagree strongly disagree

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