SUSTAINABILITY BEYOND ECO-EFFICIENCY:
A MULTI-SECTORAL SYSTEMS ANALYSIS
FOR WATER, NUTRIENTS, AND ENERGY

by

Rodrigo Villarroel Walker

(Under the direction of M. Bruce Beck)

Abstract

In recent decades, efficiency has been the flagship for the achievement of environmental sustainability, but it has been demonstrated that efficiency alone is not capable of guiding technological efforts beyond fine-tuning of old schemes that are intrinsically unsustainable. Therefore, this dissertation explores the use of systems analysis, in the form of a Multi-sectoral Systems Analysis (MSA), for environmental sustainability assessment supported by a novel set of socio-ecological indicators designed using not only eco-efficiency but also eco-effectiveness concepts. For now, the focus of the MSA framework is on flows of materials (water, nitrogen, phosphorus, and carbon), and energy, as they pass through a web of processes described by a total of five industrial sectors: water, forestry, food, energy and waste management. This kind of analysis reveals the advantages of studying different substances simultaneously (N, P, C, water, and energy) in addition to interpreting them individually. The uses of the MSA framework are illustrated by a three-part case study using the Upper Chattahoochee Watershed as the system. The first part investigates material and energy flows with the purpose of gaining insight into the magnitude of these flows, thereby establishing what it is referred as the *base case*. Results show that natural flows are predominant in the water and energy cycles. Human manipulations of water are less than 30% of the amount received as precipitation, while the total energy requirement of the system is 3% of the solar input. On the other hand, the cycle of nutrients (N, P, C) is strongly related to the flows of the poultry industry, fuel consumption, fertilizer use, and biomass use. The second part of the case study elaborates a forward approach for assessing the improvement of the system, as measured by the set of indicators, prompted by the introduction of three technologies: urine separation (UST), pyrolysis of poultry litter (PLP), and pyrolysis of municipal sludge (MSP). This exercise reveals that the selection of technological solutions must consider which is the material of interest. Urine separation and municipal sludge pyrolysis were the most advantageous combination for the recovery of nitrogen, but for phosphorus, sludge pyrolysis alone appears to be adequate. The third part of the case study couples the Regionalized Sensitivity Analysis (RSA) procedure with the MSA framework as an inverse approach to identifying those parameters, and consequently those flows and sectors, that are *critical* for attaining targets defined in terms of indicators. The results indicate that to improve the performance of a select set of indicators by 30%, certain aspects of the system, such as runoff from impervious areas, emissions from coal and natural gas use, fuel consumption for transportation, and poultry litter, are *critical*. Additionally, it is shown that there are other sources of nutrients to the sewer network, besides household wastewater, that are also relevant for improving the system. The modeling platform upon which the MSA framework is built makes this a versatile tool that can be used for assessing the impact of infrastructure changes and management decisions. Moreover, in the more general context, this dissertation can be seen as a step forward towards answering questions such as how human-managed systems can become a force for good within the environment.

INDEX WORDS: nutrient cycles, urban metabolism, environmental modeling, water, eco-effectiveness, eco-efficiency, energy, regionalized sensitivity analysis, waste management, the Upper Chattahoochee Watershed, sustainability assessment, nitrogen, phosphorus, carbon, emissions, resources, Substance Flow Analysis

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Dedication

To Julia and Miguel

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Table of Contents

List of Figures

List of Tables

Chapter 1

INTRODUCTION

"The world will not evolve past its current state of crisis by using the same thinking that created the situation." Albert Einstein

1.1 Background

1.1.1 Present Environmental and Resource Challenges

The first decade of this new millennium has been characterized by dramatic changes around the globe: significant technological advancements, atypical dynamics of economic markets, increasing natural disasters, and a continuous buildup of public awareness about the effects that anthropogenic activities have on the environment. A recent work presented by Crutzen *et al.* (2007) before the US National Academy of Engineering describes urban centers as a bull grazing in a china shop — the fragile environment — consuming large amounts of resources and releasing its bodily wastes to the surroundings. With more than half of the world's population dwelling in cities, urban areas are the engine for *natural capital* consumption. World population is projected to increase to nearly 9 billion by 2050 (Annan, 2000), so that increased pressure on the already complicated dynamic between productive sectors and the allocation of resources is expected. Under current schemes of production, and the characteristics of the products (e.g. polluting cars, toxic pesticides, disposable products made of non-degradable materials), rapid population growth can lead to economic, environmental, and social stress (UN, 1991).

The United Nations in their World Water Development Report (UN, 2006) proposed a list of five challenges for life and well-being with a clear emphasis on water, food (nutrients), energy, and the role of cities:

- Protecting Ecosystems
- Water and Cities
- Securing the Food Supply
- Water and Industry
- Water and Energy

About 2.6 billion people have no access to improved sanitation, mostly in parts of Africa, Asia, and South America. Nearly a third of them, 884 million people, do not use improved drinking water sources (WHO/UNICEF, 2010). The figures vary enormously among regions and have some correlation with the level of economic development of the region, as shown in Table 1.1. Energy use per capita has a positive correlation with economic development, showing that more developed regions have a larger consumption of energy per capita. One of the issues from the point of view of future energy availability is that energy usage relies heavily on non-renewable fuels, of which over 85% is fossil-fuel based. Table 1.2 shows the proven reserves of fossil fuels, consumption rates, and the life of reserves based on current consumption rates. From the same table, it can be seen that coal is one of the most abundant resources, while petroleum and gas might be exhausted in less than a person's life time. The scenario turns even more complex when socio-political factors are introduced to the market of fossil fuels. For instance, if the US were to rely only on its own oil reserves, it would be a matter of three years to deplete them. Another relevant issue of relying on fossil fuels is the release of long-lived Green House Gases (GHG). From 1970 to 2004, GHG emissions increased by 70% (IPCC, 2007). Beyond the traditional boundaries of the energy sector, anthropogenic CO_2 and CH_4, together with other climate change drivers, such as resources over-exploitation, land use changes, and reduction of natural systems, are having dramatic effects on water and food systems. Water availability is increasing in higher latitude regions but decreasing in lower latitudes, with a higher risk of winter flooding and reduced summer flows. The effects on water quality are not well understood yet, but some work has been done on the way global climate change might affect the city-watershed system as actions are taken towards achieving a more sustainable water sector (Beck *et al.*, 2010b).

With agricultural activities using about 80% of water withdrawals, water availability and climate temperature have a direct influence over the capacity for crop production. A mere increase of 1–2°C in temperature will reduce cereal production in low-latitude regions but increase it in mid-to-high latitudes. Although crop productivity is expected to increase globally, the opposite could occur if temperature increases more than 3°C (IPCC, 2007). However, it is difficult to predict the global trend of food markets and food distribution. By 2009 there were an estimated 1.02 billion people undernourished worldwide, with more than 60% located in Asia and the pacific region. Food and fuel prices soared during the 2008 economic crisis, affecting the poor, who were obliged to change in some cases their dietary needs and food preferences to reduce expenses. Although the amount of food is enough to feed global population, food prices and the disparity of food availability around the globe results in increased under-nourished population numbers and hunger-related deaths (FAO, 2009b).

Crop prices and productivity are also a function of the accessibility of macro-nutrients for soil fertilization, namely nitrogen (N), phosphorus (P), and potassium (K). Nitrogen is an abundant element in the atmosphere, typically converted into ammonia through a very energy intensive process, first separating N from other air components by cryogenic distillation and second, the Haber-Bosch process, synthesizing ammonia by a catalytic reaction of N and hydrogen — usually from a fossil fuel source. Phosphorus and potassium, both considered non-renewable resources, are obtained by mining phosphate and potash rock respectively. The

Table 1.1: Regional development indicators for water and energy compared to real GDP per capita (all data for year 2004).

Region	**Drinking Water Coverage**[a]	**Sanitation Coverage**[a]	**Energy Consumption**[b]	**GDP**[c]
Africa	62	44	4.7	1.1
Asia and Oceania	82	47	11.4	2.9
Europe	97	-	42.7	26.8
Latin America and Caribbean	91	77	14.9	4.8
North America	100	100	82.2	40.7
World	83	59	20.6	6.8

[a] percent, source UNEP (2007).
[b] MWh per capita, source EIA (2010).
[c] thousands US$ per capita reported as 2005 US dollars, source USDA (2009).

main two uses of these minerals are soil fertilization and animal feed. P is more abundant than K with conventional reserves in the order of 12000 and 8400 million tonnes respectively. However, the extraction and utilization rates of the two are quite different, resulting in an estimated reserve life of only 88 years for phosphorus and 325 years for potassium (Roberts and Stewart, 2002).

The previous discussion highlights water, food, and energy security as significant challenges for life and human development; therefore, this dissertation has the intention to address questions about sustainability in a technical and quantitative manner with a focus on these critical resources, more specifically water, nitrogen, phosphorus, carbon, and energy. Although not part of the scope of this dissertation, it is important to acknowledge the complexity that aspects such as scarcity and growth add to future planning and forecasting. It is in these

Table 1.2: World and US fossil fuel reserves and annual consumption for 2004 — data source (EIA, 2010).

Fuel	**Reserves**[a]		**Consumption**[a]		**Reserve life**[b]	
	World	**US**	**World**	**US**	**World**	**US**[c]
Coal	908092	245847	5000	998	182	246
Petroleum	1265000	21000	29565	7300	43	3
Natural Gas	6300	195	98	22	64	9

[a] Coal in 10^6 metric tonnes, petroleum in 10^6 barrels, and natural gas in $10^{12}\,m^3$ at standard conditions. Consumption is annual.
[b] Reserve life in years is calculated assuming consumption remains constant.
[c] Reserve life assumes that only internal reserves are used to satisfy internal consumption.

terms that some economists debate the challenges for intergenerational equity, and how finite resources might prevent a desirable non-declining well-being (Pezzey and Toman, 2005).

1.1.2 Introduction to Sustainable Development

Despite the fact that the present dissertation is not devoted to develop concepts on sustainability, this section is presented as a preamble to transmit the mental attitude under which the methodologies elaborated herein are conceived. This section discusses different angles of sustainability and highlights the importance of cities in this context.

Over the last century, the notion of *Sustainable Development* has grown in different fields of science and popular knowledge in a rather intuitive manner. Formal and informal literature shows that numerous attempts have been made to reach a practical and generalized definition of sustainability. The most commonly used concept is extracted from the Brundtland report (WCED, 1987),

> *"Meeting the needs of the present without compromising the ability of future generations to meet their own needs."*

The Brundtland definition refers mainly to the consumption of resources and the existing worry with respect to the availability and quality of resources for future generations. Poor management of renewable resources and the depletion of those non-renewable resources for which no economically feasible substitute has been found, are only part of the concern expressed in this concept. A possibly more specific concept, because it is not based on speculations about "future needs", is the one presented by Solow (1993),

> *"... an obligation to conduct ourselves so that we leave to the future the option or the capacity to be as well off as we are."*

For a better discussion of what the latter definition calls *the capacity*, it is useful to introduce the notion of *Capital Stocks*, which are usually segregated into economic, technological, natural, and human capital, see for instance Ayres *et al.* (2001). Solow's concept of sustainability could be interpreted as the desire for maintaining the overall capital (capacity) in time, at least at the same level as now, so that the depletion of one form of capital can be compensated by increasing another form. As an example, one could think of the mining industry where the natural capital is depleted, a mineral ore for instance, but part of the revenue generated from the commercialization of the mineral is invested to promote more advanced technologies for either enhancing the mineral extraction from exhausted mines or, even better, substituting the need of a presumably non-renewable resource by a renewable one. However, this so called compensation cannot be applied as straightforwardly to less tangible capitals, such as fauna and flora diversity. It would be very difficult to establish the equivalent of the existence of an endangered species in terms of another capital. The role of animal and plant species within natural ecosystems is usually recognized but often not fully considered and, moreover, according to deep ecologists, western culture legitimizes the domination of nature rather than promoting *biocentric egalitarianism* (Mebratu, 1998). Capital substitution is related to the concepts of *weak* and *strong* sustainability. Strong sustainability suggests maintaining at least equal amounts of different types of capital in time, while weak sustainability refers to the increase of one or more stocks by diminishing the rest, assuming that forms of capital are exchangeable (Ayres *et al.*, 2001; Chen and Beck, 1997).

All definitions of sustainability express, explicitly or implicitly, concern about the accelerating deterioration of the environment and the potential consequences for economic and social development. This three-dimensional character, also called as the three pillars of sustainability, was also recognized in the Bruntland report where the triple-bottom line — {*environmentally benign*}, {*economically feasible*}, and {*socially acceptable*} — was described as the baseline for a sustainable development. The impairment of one of these aspects results in the imbalance and decline of the other two aspects. For instance, a contaminated environment will result in worsening human well-being aspects, since it represents a threat to health. Similarly, a poor economy may result in improper infrastructure for waste treatment and disposal, increasing the chances for environment pollution. The economic dimension of sustainability is usually straightforward; if a system generates profits then it is sustainable from the economic point of view. However, Solow (1993) suggested a dual connection between environment and sustainability with economic connotations. A system can profit from the future by burdening the environment and the cost associated with the environmental burden could also be transferred to other systems, so that the situation is not really sustainable. The previous assertion implies a critical role for public policy and ethics (Mebratu, 1998), with consequences for systems improvement. Which dimension of sustainability, as contemplated by the *triple-bottom line*, is more important? Which dimension needs to be improved first?

Social involvement is critical for a transition towards more sustainable schemes, especially because people are directly involved in resource consumption. Huesemann (2004) indicated that western society cannot be sustainable if social structure, life-style, and values are not subject to evaluation and change. The role of different actors, i.e., the general public, government, and private enterprise, towards this change can be identified after segregating products into two kinds (McDonough and Braungart, 2002): (i) products of consumption, that is directly consumed by people, such as water, food, shoes, and clothes, and (ii) products of service, such as fuels, cars, and televisions sets, which is applicable when the user is actually seeking a service (transportation, entertainment, constant temperature at home, etc.). The general public has a clear influence on the former type of product, but corporations can play a key role making service products more sustainable. At many levels of society, decision-making is influenced by society through political action and public choice. Political willingness is crucial (Annan, 2000), but in some cases it could be driven by interests different to those aligned with population well-being. Public acceptance and choice are to a large extent subject to public perception and awareness, see for example Osidele (2001) and Larsen and Lienert (2007). Promoting social learning and participatory involvement typically reduces social-cultural difficulties in the implementation of new technologies that often involve change and adaptation of the public's behavior (Balkema, 2003; Kates *et al.*, 2001). In order to achieve an effective knowledge transfer to society it is of primary importance for scientists and engineers to understand public beliefs, fears, and desires. Information technology fits perfectly as an structured vehicle to increase and improve technical knowledge diffusion while facilitating stakeholder understanding on the implications that behavior change have on the performance of a system (Mihelcic *et al.*, 2003; Demir, 2010).

Walsh *et al.* (2006) proposed a set of sustainable requirements for a satisfactory urban life with regard to energy and water use, food consumption, non-renewable resources use, transportation and housing needs, and waste management. Their estimations are based on

(i) resource availability in the present and for the future, (ii) levels of resource use, and (iii) resource use not only for survival but for the maintenance of productive and satisfying lives. The study reveals the disparity in the perception of requirements around the world. For instance, stronger economies perceive that a higher level of consumption is required compared to less developed regions, demonstrating that establishing a sustainable state is quite dependent on social behavior and societal structure.

Within the popular knowledge context, sustainability is mostly viewed as a topic exclusive to environmental matters and assumed to be in disagreement with economic development. However, it has been demonstrated that innovative and smart ideas can be environmentally friendly and economically feasible at the same time (McDonough *et al.*, 2003; Larsen and Lienert, 2007). It is often suggested that a sustainable process or system should aim at zero emissions and zero waste generation, thus, optimization of processes is often carried out with this goal. However, if optimization is performed without a chain-oriented view, the procedure is flawed in the sense that unexpected environmental burdens could be transferred to other systems. This case has been illustrated for a Vinyl Chloride Monomer process where the minimum global environmental impact corresponded to an optimal point of dichloroethane emissions different to zero, and reducing emissions levels below that point resulted in increased waste generation due to the trade-offs between inputs and outputs (Azapagic and Clift, 1999). Therefore, a possible approach to less unsustainable processes could be improving efficiency with the objective of closing the gap between system's releases and the capacity of the environment to "digest" those releases, usually described in terms of ecological resilience — the ability of the environment to *attenuate* and *absorb* perturbations (Beck, 2005) — and carrying capacity — the amount of activity that can take place without detrimental effects to the environment (Arrow *et al.*, 1996). However. the practicality of this approach is subject to the uncertainty associated with the definition of the "digestibility" capacity. In addition to a chain-oriented approach, life-cycle thinking can bring insight into the sustainability of a system particularly if other stages besides the operational, such as construction and decommissioning, are thought to be relevant; but then, if a system is really sustainable by generating wealth while also improving social and environmental conditions, why would one want to dismantle such a system?

The conclusion that can be drawn from the different definitions and descriptions discussed herein is that the concept of sustainability varies from one field to another and is typically inexplicit. Some have argued that the lack of a concise and non-manipulable concept represents a real threat to the practical aspect of sustainability (Wall and Gong, 2001). On the other hand, this vagueness makes sustainability concepts adaptable and suitable for interpretation under new or unexpected situations. In general terms, it can be said that the definition of sustainability faces three major challenges,

- Sustainability concepts are heavily anthropocentric, often ignoring the existence and the well-being of other species and wilderness, except for the benefit of human beings (Batterham, 2003).
- There are implicit difficulties in defining what is considered sustainable now and, even more hard to accomplish, what would be understood as sustainable in the future.
- Sustainability analysis needs to be approached in a holistic way as opposed to localized to avoid sub-optimal solutions. This calls for a more multidisciplinary formulation that includes the triple-bottom line aspects and a chain-oriented concept as well.

Cities and Sustainability

The role of urban areas in the present and future challenges for sustainability was already mentioned in Section 1.1.1. On many occasions, the behavior of cities has been compared to that of biological organisms, revealing after close examination that some elements of the urban setup, such as road infrastructure and electrical cable length, shows resemblance to the power law where metabolic rate, M, defined as the power required to sustain the organism, scales as $M \propto {B_w}^{3/4}$, where B_w is body mass. However, other processes, such as crime, wealth, and innovation, all related to human needs and social dynamics, grow at a faster pace (Bettencourt *et al.*, 2007). This is in agreement with the statement that the control that humans exert over biochemical reactions differentiates city behavior from that attributed to living organisms (Kaye *et al.*, 2006). Despite the differences, and the difficulties that these create for growth prediction, the analogy of cities as living things is valid in the sense that resources are consumed, work is done — thermodynamically speaking — and wastes generated.

In the 1990's, the City of Phoenix, with a population of just over 3.6 million, consumed nearly $25 \times 10^3\ \mathrm{t\,y^{-1}}$ of nitrogen (N) in food, and released more than $72 \times 10^3\ \mathrm{t\,y^{-1}}$ of N to the atmosphere in different chemical forms. Half of those emissions are attributed to combustion. To put these numbers in perspective, the magnitude of nitrogen entering the system through deposition and fixation, which is typically the major input to a natural system, amounts $11 \times 10^3\ \mathrm{t\,y^{-1}}$. Not only nitrogen but also phosphorus and carbon are just a few materials that find their global cycles distorted and accelerated by the presence of cities (Beck and Cummings, 1996).

The quest for sustainability started, in the primitive form of survival, by securing water supplies, which explains why the largest metropolitan areas are located nearby water bodies. With sprawling settlements then came the second challenge, how to keep wastes out of cities? Water, as a transport medium, was the answer; this practice is still in use. Originally, wastes were sent to streams without prior treatment. It was only in the early 20th century that the correlation between the direct discharge of sewage into the streams and public health issues began to be recognized, leading finally to the construction of sewage-treatment facilities. As a collateral consequence of using water to convey wastes that are rich in nutrients, the perception of wastewater treatment as a process for merely removal of contaminants and pathogens and to produce clean water has shifted to a resource recovery view (Chen and Beck, 1997; Balkema, 2003; Beck, 2005). The apparent trend of actions seems to a have reactionary characteristics; systems are improved when a failure or weakness is identified, not before, possibly because there is no ultimate, and measurable, goal for sustainability. This evolutionary process towards less unsustainable states is described by Wilkinson and Cary (2002) based on the gradual historical development of agricultural systems in Australia, concluding that a sustainable system is described as the one that can adapt and respond to major disturbances, i.e., a resilient system. However, if disturbances have become more pronounced, as is happening due to climate change, a reactionary approach might not be sufficient to guarantee survival, and a more futuristic vision might be appropriate.

Computer simulations have always been useful to explore future scenarios. A study conducted by Lundie *et al.* (2004) to estimate potential environmental impacts of Sydney Water's operations as projected to 2021 compared nine different scenarios including desalination, water demand management, population behavior changes, energy efficiency, energy generation, among others. This research work clearly illustrates the environmental challenges that centralized systems have in adapting to ever growing cities, while decentralized and local water management resulted in the best scenario. Although this case focuses only on the water sector of the city of Sydney, it is easy to extrapolate the use of simulated approaches to other sectors of the city to understand the outcome of speculative scenarios. Cities, and urban areas in general, have the great opportunity, and some will say the responsibility, of overturning the current perception of cities as "a bull grazing in a china shop" into a cumulus of processes and activities that results in beneficial flows to the surrounding environment, flows that will nourish other systems instead of deplete them.

1.2 Research Objectives

Sustainability is usually expressed in terms of {*social acceptance*}, {*economic feasibility*}, and {*environmental benignity*}. This dissertation focuses on the environmental component, but acknowledges the importance of the other two. Additional discussion about the three-dimensional character of sustainability is addressed in Sections 2.1 and 7.1.1.

In order to address environmental issues in a comprehensive way, it is imperative then to consider more than one sector, i.e., more than just the water sector or the energy sector, and include the several interactions among technical sectors (Lundin *et al.*, 2000). The synergy among sectors such as the water, energy, and food industries is evident, see for example Barczak *et al.* (2005). The primary objective in this dissertation is to explore the usefulness of a systems analysis methodology in a multi-sectoral context for supporting environmental sustainability assessment. Instead of using well established methods for estimating potential damage and environmental burden, this study examines the metabolism of critical materials and energy — water, nutrients, and energy — at a socio-ecological level (Azar *et al.*, 1996). The purpose of a broad systems analysis, i.e., one that involves a chain of processes, is to avoid generating information that could lead to localized decisions, as these can erroneously indicate that an environmental issue has been removed when it is actually being exported to another sector. For instance, wastewater treatment facilities reduce potential eutrophication of receiving waters by removing nitrogen from wastewater, but it requires important amounts of energy which has an equivalent release of GHG, if that energy comes from fossil fuel sources (Deslauriers *et al.*, 2005). The Multi-sectoral System Analysis (MSA) is meant to be informative and credible even in the face of poor data or other sources of uncertainties, by implementing a sample-based technique for uncertainty analysis, namely the *Monte Carlo simulation.*

It has been demonstrated that implementing efficiency alone will not lead to sustainability in terms of the environment (Hanssen, 1999; Huesemann, 2004; Barbiroli, 2006; Braungart *et al.*, 2007), thus this dissertation aims to propose and instrument a set of macro-indicators involving not only eco-efficiency, but also eco-effective criteria. These macro-indicators have a double purpose:

(i) First, as measures of a system's performance making MSA therefore a tool capable for comparing scenarios, similar to the case explored by Lundie *et al.* (2004), and even more specific, for recording the effects that a structural change, within the system, might have on the system's behavior. In MSA, the system is represented by a web of processes and the material and energy flows interconnecting them, and a structural change, as considered by the MSA, of this web of processes can be the result of an infrastructure change, a management decision, or the implementation of a new technology.

(ii) Second, as quantitative instruments for the elaboration of sustainability goals. After defining targets based on, for instance, regional priorities or public desire, the Regionalized Sensitivity Analysis (RSA) procedure can be employed to assess the reachability of those goals and identify which processes, flows, or structural changes are key for meeting them.

After describing cities as a focal point for sustainability considerations, it is desirable to present this work as an initial move towards the vision of turning urban-rural systems into forces for good in the environment. With that in mind, one can pose two questions: what structural changes, within the anthropogenically controlled cycles, are necessary to achieve this? What would be the most adequate sequence of steps to perform these changes? This dissertation illustrates the use of the MSA+RSA framework as a sustainability assessment tool under uncertainty with the hope that it would serve beyond solely the role of being informative to be of value for actual decision-making.

1.3 Selected Approach

This section describes in general terms the different methods and approaches that are used to respond to the research objectives of this dissertation. The combination of a multi-sectoral approach with Substance Flow Analysis (SFA) and Regionalized Sensitivity Analysis (RSA) for the assessment of a system under measures of eco-effectiveness concepts, makes this work a novel attempt, and a considerable enterprise, in the field of sustainability evaluation of human systems. Chapter 2 complements this assertion and puts together part of the knowledge behind the methodologies employed herein.

1.3.1 The Conceptual Picture of the System

An urban-rural system is segregated into five different industrial sectors that provide services to the population:

- Water sector
- Food sector
- Forestry sector
- Energy sector
- Waste management sector

The Substance Flow Analysis (SFA) methodology is used to track inputs, outputs, and conversions in chemical form or phase of water, nitrogen, phosphorus, carbon, and energy across the five sectors, see for example Antikainen *et al.* (2004). This is referred to as the Multi-sectoral Systems Analysis (MSA) that is based on process flow diagrams elaborated for each sector. The approach of using Flow diagrams is well structured and suitable for describing the fate or routes of substances and facilitate the elaboration of inventories of material. Methods such as Life-Cycle Assessment (LCA), SFA, Material Flow Analysis (MFA), and exergy analysis use flow diagrams extensively.

1.3.2 How to Measure "Good" rather than "Less Bad"

It is precisely because of its conceptual ambiguity that measuring sustainable development is a great challenge. Decision-making, management, and research are among the most important reasons for having sustainability measures (Parris and Kates, 2003). Based on the process flow diagrams mentioned before, it is possible to elaborate a set of eco-efficiency and eco-effectiveness indicators that account for the resources consumed, products generated, wastes disposed, and emissions released. Therefore, these indicators fall under the categories of societal activity and environmental pressure indicators (Azar *et al.*, 1996). Eco-effectiveness, as such, has never been instrumented in a quantitative manner, but it is believed to be a necessary step to start assessing and improving systems towards goals that are more informative about sustainability than damage-oriented or other environmental quality indicators. Although these types of indicators are widely used, Azar *et al.* (1996) explains two reasons why they fail to provide a timely warning of future environmental issues:

- First, because there is usually a time delay between the "transgression" and the corresponding environmental harm. Actions supported by indicators that reflect environmental *state*, e.g. global temperature and lake nitrogen concentration, might be too late or require significantly more efforts to reverse the damage. The *state* might also reflect activities that took place in the past.
- Secondly, ecosystems and natural cycles are quite complex, making difficult an effective prediction of what possible effects an activity has on the environment, let alone determining where and when the environment will make evident its damage.

1.3.3 From Conceptual to Representative Art

The flow diagrams will serve as the blueprint for developing the mathematical expressions representing processes and the corresponding interconnections of material and energy flows.

The equations involve a large number of parameters that define process rates and the overall behavior of the system. The specific values of these parameters depends on population consumption patterns, management choices, and process kinetics. The behavior of the system is also subject to forcing functions and input data, such as climate conditions and region properties (e.g. land use). Being adaptable, through the ability of adjusting parameters to region-specific conditions, makes the simulation framework applicable to almost any system. However, parameters contain a degree of uncertainty as the result of measurement procedure errors, instrument errors, or simply random errors, and the propagation of this uncertainty must be reflected in the output of the simulation as this information is advisable for a robust decision-making process.

As mentioned before, the balance of material is carried out for water, nitrogen, phosphorus, and carbon following the SFA methodology, requiring vast amounts of data. The collection of data is mostly supported by reports issued by government agencies, global organizations, and university extensions, and peer-reviewed journals. Regional information is desirable, but in the face of the lack of specific information, national or global data are introduced. This is also a source of uncertainty. At this point, the possible output of such a systems analysis is basically for accounting purposes, that is, identifying important flows, stores, emission sources, waste sources, and resources demand. Indicators add another dimension to the study by making possible the assessment of the system's performance. Eco-efficiency indicators are calculated based on how well resources are used and how much product, waste, and emissions are generated from their use. On the other hand, eco-effective indicators provide a measure to compare the system and sustainability, thus requiring the definition of a *reference state*. Once indicators are defined, the usefulness of MSA can be tested in a practical way, using a real system case study (the Upper Chattahoochee Watershed), by investigating how the performance of the base case is compared to scenarios derived from different combinations of three relatively new and innovative technologies (urine separation, poultry litter pyrolysis, and sludge pyrolysis).

1.3.4 Credibility

The *Monte Carlo simulation* allows estimating the most likely values of material and energy flows, and subsequently the resulting value of indicators, accounting with this for the uncertainty associated with each parameter. Rather than simplifying the structure of the system as a way to decrease potential sources of uncertainty from parameters, the MSA+RSA framework judges which elements of the model are not relevant for the particular indicator. If uncertainty is not ignored, parameter-intensive models can result not only in a more comprehensive systems analysis but also in more informative results for management, policy, and decision-making in general. Environmental models have always faced the lack of credibility, particularly among the common citizen, given that nature and natural processes are quite complex.

Summarizing, a modeling approach, as opposed to a pure material and energy accounting exercise, offers a flexible framework that allows for several benefits including multiple scenario assessment and propagation of uncertainty. The RSA component in this research adds *practical credibility* to the model results and interpretation, which later can lay the foundations for evaluating the *reachability* of sustainability goals (Osidele, 2001).

1.4 Structure of the Dissertation

This dissertation is organized into seven sections. The present chapter describes some of the major challenges that the human race is currently facing, how sustainability is understood in different contexts, and demonstrates that urban areas are central to the the topic of sustainability. Chapter two presents a literature review of the different conceptual approaches and tools for environmental assessment. Chapter three explains how the Multi-sectoral Systems

Analysis (MSA) is structured, gives details for each sector, elaborates on the set of eco-efficiency and eco-effectiveness indicators, and discusses the implementation of RSA within the simulation platform. The MSA usefulness is tested in a three-part case study. In Chapter four, the *base case* scenario is established using the Upper Chattahoochee Watershed as the *system* with data corresponding to year 2000. Flows of water, nitrogen, phosphorus, carbon, energy are examined and the magnitude of these flows is discussed. Chapter five complements the previous chapter by introducing the use of indicators and assessing the performance of the system before and after implementing three technologies: urine separation, poultry litter pyrolysis, and municipal sewage sludge pyrolysis. Chapter six completes the triplet of case studies by employing RSA as the procedure for testing the reachability of sustainability goals and identifying the key processes for meeting these goals. Conclusions, recommendations for future research, and final remarks are compiled in Chapter seven. Appendix A contains a list of abbreviations and symbols. Appendix B presents a list of parameters and inputs used in the MSA model together with their identification code. Appendix C shows an schematic representation of the model code structure (developed in MATLAB®) and the interaction between the procedures of MSA and RSA. Appendix D describes, in a visual manner, the mathematical behavior of indicators as a way to increase the understanding of the performance of the system and interpretation of results.

Chapter 2

LITERATURE REVIEW

"Under the existing paradigm of manufacturing and development, diversity — an integral element of the natural world — is typically treated as a hostile force and a threat to design goals." W. McDonough and M. Braungart

The approach described in Section 1.3 is based on a number of concepts and methods that are explained in this Chapter. First, some of the tools used for sustainability assessment are described and compared to the one selected for this research, Substance Flow Analysis. Second, given that the design of a set of sustainability measures (indicators) based on eco-efficiency and eco-effectiveness concepts is part of the scope, these two terms are explained and contrasted. Next, the complexity of the nutrients of interest (N, P, and C) and the fact that these are relevant for all the five sectors, makes it necessary to draw a detailed picture of the interactions among biomass, soil, hydrological and atmospheric processes, land use, and the nutrient cycles. The other two species considered in this work (water and energy) are better described by their respective sector and hence explained in Chapter 3.

2.1 Sustainability Assessment

There is a broad spectrum of approaches for sustainability assessment, designed for different goals and scopes. Environmental analysis tools can be characterized based on the description presented by Finnveden and Moberg (2005), summarized in Table 2.1. The focus of a tool might be of an analytical or procedural nature. The former is dedicated to the technical aspect of the analysis, e.g Substance Flow Analysis (SFA), while the latter is centered on the procedure and its interaction with its societal and decision context, e.g. Environmental Impact Assessment (EIA). Analytical tools can also be implemented within procedural tools. The character of the tool is also important to determine the context in which a tool can be used; descriptive tools are used for retrospective analysis to examine the attributes of a system at a specific time. On the other hand, change-oriented tools are best suited for scenario comparison. For instance, based on Table 2.1, SFA can be classified as a tool with an analytical focus, with mostly an environmental impact, where the object is a substance, and it could have either a descriptive (material accounting) or a change-oriented character (scenario assessment). In addition to the classification presented in Table 2.1, assessment tools can vary according to their specific **purpose** (e.g. population wealth, land productivity, and clean air), **means** (e.g. equity, education, and technology), and **motivation** (e.g. measuring progress towards a goal, identifying a range of possibilities, providing guidance for decision-making).

Table 2.1: Typical characterization of environmental systems analysis tools after Finnveden and Moberg (2005).

Focus	**Impacts**	**Object**	**Character**
Analytical	Environmental	Policies, Regulations	Descriptive
Procedural	Economic	Regional, National	Change-oriented
	Social	Organizations, Companies	
		Products, Services	
		Materials, Substances	

Environmental analysis tools can also be segregated based on their relevance along the chain of production, or life-cycle of the product or service. As suggested by Guinee (2001), tools are classified as *transverse* or *longitudinal*. The former is typically associated with a single step of the chain, while the latter has the capability for analyzing one or more steps. For example, tools such as Technology Assessment (TA), Environmental Impact Assessment (EIA), Environmental Management Systems (EMS), and Risk Assessment (RA) are referred as *transverse* because the focus is typically one stage at a time (e.g. raw material extraction, production, or transportation). On the other hand, tools such as Life-Cycle Assessment (LCA), Substance Flow Assessment (SFA), and Exergy Analysis, are known as *longitudinal* because they can include the whole chain of processes. In the next section, a discussion is initiated with regard to sustainability indicators as a preamble for the following sections that include a general review of the most used sustainability assessment tools.

2.1.1 About Indicators

The way in which the performance of a system is measured is relevant for addressing any discussion about sustainability, but despite the numerous attempts to define a universally accepted set of indicators for sustainable development, this has not been achieved. Most of the indicators found in literature are useful for comparing different states or situations, but it is less common to find indicators that measure the degree of deviation from a desirable state (a "sustainable" state). Two examples of efforts to create unambiguous indicators are: (i) exergy measures, by representing the deviation from an equilibrium state, usually the surrounding environment (Wall and Gong, 2001), and (ii) the eco-indicator99 which relies on values of acceptable resource consumption and emissions rates for generating a weighting factor for impacts categories (e.g. global warming, ozone depletion, and eutrophication), that can later be interpreted as a measure of the departure from sustainability (Goedkoop and Oele, 2004). To clarify the role of a measure, Sahely *et al.* (2005) discuss the difference between indicators and criteria, concluding that the first are mostly used for performance monitoring while the second compares the system performance versus a *reference state*. The lack of consensus for a universal indicator or criteria system is thought to derive from (i) definitional ambiguity, (ii) great number of purposes, and (iii) unclear terminology, data, and measuring methodology (Parris and Kates, 2003). Regarding the latter, there has been important improvement in specifying more rigorous methodologies in recent years. For environmental assessment, methodologies such as Life-Cycle Assessment (LCA), exergy analysis, and Material Flow Analysis (MFA) count nowadays with a vast literature that shows the ongoing effort for unifying criteria for implementation and analysis. See for example (Guinee, 2001; Wall and Gong, 2001; Brunner and Rechberger, 2003).

For technology screening, Balkema (2003) includes indicators that involve the three aspects of sustainability by using traditional cost estimation, optimal resource utilization and emissions levels, and qualitative indicators for the social dimension (see Table 2.2). Although the contribution of social indicators is quite subjective it is preferable to include social aspects to some extent rather than just ignore them. Additionally, she introduces a *functional* component that relates end-user needs to the characteristics of a certain technology, such as requirements for technology performance, requirements of maintenance, robustness, and reliability. A positive aspect of the set of *functional* indicators is their easy conversion to monetary terms. Similar to many others studies, Balkema recurs to the use of a weighting procedure that aggregates economic, environmental, social, and functional metrics to obtain a single index. This approach eases the decision-making process and provides great advantage when the procedure is followed by an optimization routine. Aggregation could also be used to express local preferences or priorities by assigning a larger weight to those indicators that are more critical or relevant for the system. However, the weighting procedure is always associated with subjectivity and the potential opportunity for manipulation, while a single index can lead to overlook trade-offs among indicators and losing valuable insight that can otherwise be derived from a multi-objective approach. It is therefore recommended to extract information and draw conclusions at the various stages of the procedure.

There are several attempts to monetize environmental indicators as a way to improve their incorporation into economic assessment tools. Initially developed for analyses in the Swedish context, *ecotaxes* aims to establish valuation weighting factors for environmental emissions based on the taxes associated with the emission itself or the material that generates the emis-

Table 2.2: Indicators for the Domestic Water System as proposed by Balkema (2003) classified by their sustainability area of focus.

Functional	**Economic**	**Environmental**		**Social-Cultural**
		Emissions	**Resource use**	
-Adaptability -Maintenance -Reliability -Robustness -Waste	-Investment cost -Operation and maintenance costs	-Untreated wastewater -Treated wastewater	-Energy -Land space -Nutrient recovery -Water	-Acceptance -Expertise -Institutional requirement -Public participation -Sustainability behavior

sion (Eldh and Johansson, 2006). For example, taxes on nitrogen fertilizer can be translated into *ecotaxes* for nitrogen emissions from fertilizer application. However, taxation varies from among nations posing a challenge in the case of those emissions that have a global impact, such as NO_2 and CO_2, associated with acid rain and global warming respectively. A comparable example is the Environmental Pollution Cost (EPC) initiative developed for Canada. It is an approach based on the cost derived from environmental remediation, compensation for environmental damage, or prevention of emissions or discharges, see for example Rosen and Dincer (1999). Nevertheless, it seems that the translation of environmental issues into a currency form is more appropriate if applied to environmental impacts that are normally contained at the local level, as it is the case for eutrophication.

It is also important to mention that indicators are susceptible to spatial scale, e.g. local, regional or global. Parris and Kates (2003) performed a thorough review to describe efforts ranging from global to local scales summarizing a total of twelve initiatives with different scales, scopes, approaches, motivations, and methodology. The initiatives are presented in a condensed way in Table 2.3 to illustrate the difference between how relatively large-scale systems (e.g. neighborhood, city, watershed, or nation) differ from process unit scale analysis (e.g. combination of process units part of the domestic water system after, Balkema (2003)).

Table 2.3: Summary of different initiatives for indicators development at the global and local context after Parris and Kates (2003).

Descriptive name	**Indicators**	**Aspects Covered**	**Scale**
United Nations Commission on Sustainable Development	58	Social, environmental, economic, institutional	Global analysis at a country level
Consultative Group on Sustainable Development Indicators	46	Social, environmental, economic, institutional	Global analysis for a group of 180 Countries
Wellbeing Index	Composite index from 88 indicators	Human wellbeing (health, population, wealth, knowledge, community and equity) and Ecosystem Wellbeing (land, water air, species, and resource use)	Global analysis for a group of 180 Countries
Environmental Sustainability Index	Composite index from 68 indicators	-Global stewardship (participation in international collaborative efforts to reduce greenhouse gas emissions, and transboundary environmental pressures) -Environmental systems (air quality, water quantity, water quality, biodiversity, and land) -Reducing environmental stresses (air pollution, water stresses, ecosystem stresses, waste and consumption pressures, and population growth) -Reducing human vulnerability (basic human sustenance and environmental health) -Social and institutional capacity (science and technology, freedom to debate, environmental governance, private sector responsiveness, and eco-efficiency)	Global analysis for a group of 148 Countries

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Descriptive name	**Indicators**	**Aspects Covered**	**Scale**
Global Scenario Group	65	International equity, national equity, hunger, energy use, water use, deforestation, carbon emissions, sulfur emissions, and toxic waste.	Global analysis at a country level
Ecological Footprint	Composite index	Croplands, grazing lands, forests, fisheries, infrastructure, and fossil fuels	Global analysis at a country level
Genuine Progress Indicator	Composite index	Economic performance, economic contributions of household, volunteer work, crime, pollution, and family breakdown	National: United States
U.S. Interagency Working Group on Sustainable Development Indicators	40	Social, environmental, economic	National: United States
Costa Rica System of Indicators for Sustainable Development	-	Social, environmental, economic	From district to National: Costa Rica
Boston Indicators Project	159	Civic health, culture, economy, education, environment, housing, health, safety, technology, and transportation	From the neighborhood level to metropolitan area (specific for Boston)
State Failure Task Force	75	Based on 127 *state failures* events (wars, genocides, disruptive regime crises, etc) resulting in indicators related to social, economic, political, and environmental aspects	Global analysis at a country level

Continued on next page

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Descriptive name	**Indicators**	**Aspects Covered**	**Scale**
Global Reporting Initiative	-	Social, economic, and environmental	Global analysis at the corporate or organization level

2.1.2 Life cycle assessment

Life Cycle Assessment (LCA) is a method designed to estimate the potential environmental burden associated with a product, service, or activity in the form of emissions, resource consumption, or intervention. Potential environmental burden in this context refers to the capacity for generating harmful environmental consequences. LCA is often called a "cradle-to-grave" systems analysis tool, thus chain-oriented, aiming to include from raw material acquisition — extraction from the environment — through production, use and disposal. It is an analytical tool that can be used in a retrospective and prospective manner. LCA has been mostly used for product-focused studies, but in recent years its applicability for process screening, design, and optimization has been tested (Azapagic, 1999). Its application can be extended to monitoring, process improvement, and benchmarking, if implemented on a continuous basis as a management tool (Guinee, 2001). LCA, which is one of the most documented analytical tools for environmental assessment, is being supported by the International Organization for Standardization (ISO) by developing the ISO 14040 series in an effort to unify criteria and standardize the LCA procedure. Other agencies such as the United States Environmental Protection Agency (USEPA) and the United Nations Environment Programme (UNEP) in conjunction with the Society of Environmental Toxicology and Chemistry (SETAC) have issued comprehensive documentation to promote its use (UNEP, 2005; USEPA, 2001).

The LCA methodology is comprised of four stages as shown in Figure 2.1: (i) Scope and goals definition, (ii) Life-Cycle Inventory (LCI), (iii) Life-cycle Impact Assessment (LCIA), and (iv) Interpretation and Improvement. The Scope and goals is one of the most important as it describes the system in terms of its boundary definition and functional unit selection. In this context, boundary selection refers not only to the chain of processes involved but also to the phases of the process or product life cycle. LCA studies typically exclude the design phase, since it is considered to have negligible contribution (Rebitzer *et al.*, 2004), thus focusing, on material extraction, manufacturing, packaging, transportation, use, and disposal. The functional unit is the basis on which results will be presented and compared. A typical example is found in the evaluation of packing material with different characteristics but with the same function, $1\,m^3$ of packed product. In the case of a process, the functional unit could be defined as a mass or volumetric unit of product. LCI includes data collection and estimation of the inputs and outputs attributable to a product or a process through its life cycle, namely raw material, energy, emissions, wastes, and products. This phase, one of the most challenging phases of a LCA, involves the always time-consuming task of gathering data which have to be in accordance with the level of detail of the study. Often data are inexistent or are subject to proprietary rights, and when found, data are sometimes poor organized, outdated, and even specific to a region or country. LCI also involves a normalization step which relates in a quantitative manner data collected to the functional unit.

Life-cycle Impact Assessment (LCIA) is usually referred to as the core stage in LCA, in which the practitioner associates emissions with one or more environmental issues, called impact categories. In general, LCIA involves the following steps:

Classification: inventory data — inputs and outputs — are assigned to an *impact category*, for instance, global warming, ozone depletion, acid rain, resources depletion, or aquatic eutrophication.

Characterization: emissions are calculated to the same unit and summarized within each impact category, for example, methane, carbon dioxide and carbon monoxide are grouped as GHGs, responsible for global warming.

Valuation or Aggregation: integrates impacts in a single ranking function for direct comparison of alternatives. Eco-indicator99 (Goedkoop and Oele, 2004), IMPACT 2002+ (Jolliet *et al.*, 2003), and EDIP97 (Wenzel *et al.*, 1997) are just a few examples. Previous experiences have indicated that aggregation of life-cycle indicators based on different methods can lead to contradictory conclusions (Dreyer *et al.*, 2003).

Interpretation and Improvement: as a function of the information yielded during each of the previous steps, the practitioner may draw partial or final conclusions. This step, initially not part of LCA, was included to orient LCA studies towards improving the environmental performance of a system rather than evaluating its status-quo (Baumann and Tillman, 2004). The importance of the interpretation has to be validated through sensitivity and uncertainty analyses accounting for the variability of the data and information used.

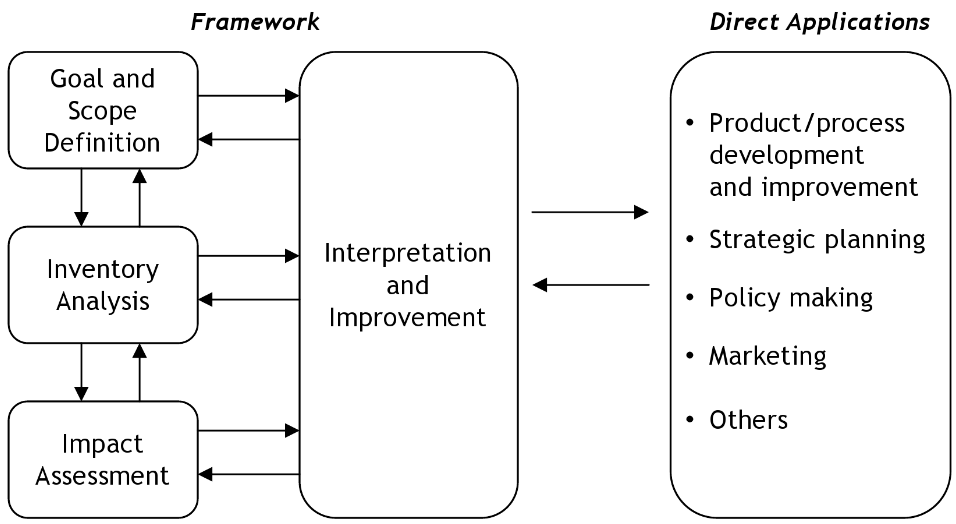

Figure 2.1: Schematic representation of the Life-Cycle Assessment Procedure and general applications.

The philosophy behind LCA has been extrapolated from the environmental realm to include economic and social aspects. Life Cycle Costing (LCC), originally proposed by the Federal Energy Management Program (Fuller and Petersen, 1995), was developed as a tool to account for the monetary cost of a product or a service along its whole life cycle (see for example, Friedrich-Wilhelm (1999)). Life-cycle cost (LCC), together with Cost Benefit Analysis (CBA) and Total Cost Assessment (TCA), is one of most widely used economic assessment tools. More in its infancy stage, Societal LCA (SLCA) is designed to gauge the geographic-specific social benefits of a product compared to another by calculating the employment hours generated in each scenario and comparing this to the benefits that arise from those employment hours, such as housing, health care, and education (Hunkeler, 2006).

The life cycle approach aims to reveal trade-offs that would remain otherwise hidden, since sustainability issues can be exported in time and space. For instance, if ethanol derived from corn is used to replace current U.S. gasoline demand, 100% of all U.S. agricultural land would be required for corn crops, leaving no land for food production or to maintain natural ecosystems (Huesemann, 2004). However, there are aspects that are still difficult to assess and measure. This is the case for technologies such as wind and hydropower, which might have a negative effect on wildlife. The LCA methodology aggregates emissions and wastes throughout the chain of processes based on their chemical properties, making difficult to address local environmental impacts and spatial variability. On occasion, the practitioner can identify the origin of certain discharges but typically cannot reveal the specific damage at a location. Therefore, LCA is not a site-specific tool and has no prediction power over the fate of substances. Recent studies have combined LCA and Risk Assessment, e.g. (Sonnemann, 2002), to estimate damage to health and environment generated by process chains, making it possible in this way to estimate a more realistic environmental impact, considering local conditions that can enhance or otherwise buffer the effect of emissions or discharges (Gasafi *et al.*, 2004).

2.1.3 Exergy Analysis

Wall and Gong (2001) suggested that no system is sustainable if resources are not renewed at least at the same rate as they are consumed, with the implicit message that renewed resources have enough potential to replenish what is being consumed. *Exergy* has been proposed as a single indicator to account for resource consumption and efficiency. The approach of exergy analysis is based on the second law of thermodynamics that accounts for the work potential of a system relative to a reference state. In a closed system, a real process will always show that the total input exergy exceeds the total output exergy due to irreversibilities within the system. The first law of thermodynamics states that mass and energy is always conserved irrespective of its form, but by introducing the concept of entropy it is possible to account for the quality of the flow, since not all forms of energy or mass can be used to generate work or heat. In this sense, the exergy analysis is capable of informing about not only the quantity of energy used but also the quality of the remaining energy with respect to a defined equilibrium state.

Exergy analysis has typically been implemented in *Design for the Environment* strategies with a process as the object of study (Rosen and Dincer, 1999). Based on the classification presented in Table 2.1, exergy analysis is an analytical tool that can be used in a retrospective and prospective manner, with the advantage that all aspects of the system can be aggregated into a single quantitative indicator. Exergy has been implemented as an indicator of resource and energy consumption especially in the area of mineral extraction and recycling (Finnveden and Ostlund, 1997; Michaelis and Jackson, 2000), fossil fuels and energy (Lior, 2002; Bargigli *et al.*, 2004), process optimization (Cornelissen and Hirs, 1997, 1998), and river water availability (Zaleta-Aguilar *et al.*, 1998). However, exergy analyses have difficulty to differentiate between renewable and non-renewable resources, and account for the fact that the former is being replenished. Cornelissen and Hirs (2002) found that even though irreversibility cannot be used to account for renewables, exergy applied within the

LCA framework can help to quantify the consumption or inefficient use of natural resources (see also Finnveden and Ostlund (1997).

Sustainability assessment by exergy analysis can express quantitatively the degree of threat of disequilibrium of an emission with respect to a reference state, but it does not offer information about the specific environmental impacts and health effects associated with the system's inefficiencies (Rosen and Dincer, 1999). In the task of communicating results to stakeholders, i.e. all people or institutions involved directly or indirectly to the system, it is challenging to translate exergy results into known environmental issues such as global warming, eutrophication, or acid rain. Therefore, some studies have suggested that exergy analysis should be used in conjunction with other economic and environmental assessment methodologies (Hammond, 2004).

2.1.4 Material flow analysis

Material Flow Analysis (MFA) explores the mechanisms associated with material transformations and material flow through socioeconomic boundaries, most of the times at the national or regional level. MFA is comprised of a suite of methods with different objects in focus. Some of these methods are: Substance Flow Analysis (SFA), Total Material Requirement (TMR), and Material Intensity Per Unit Service (MIPS). MFA methods are of an analytical nature and can be used in both descriptive and change-oriented studies. However, TMR and MIPS are usually applied to retrospective studies while SFA studies have been found to be useful in both retrospective and prospective studies (Finnveden and Moberg, 2005).

TMR is a highly aggregated indicator that reflects the cumulative volume of primary materials extracted from nature to support the economy of a nation. TMR includes both domestic extraction and material requirements associated with imports. The latter includes the so-called "hidden" flows, i.e., those extractions which are not further utilized, such as mineral overburden, processing waste, and soil erosion. MIPS is similar to TMR, but it focuses on a product or a service. MIPS quantifies the material intensity — mass per unit of product — by aggregating the overall material input used to manufacture a product or provide that service. The material input is calculated in five categories: non-biotic raw materials, biotic raw materials, water, erosion, and air. To some extent, the MIPS method works as an indicator of manufacturing or process efficiency.

SFA is especially designed to track substances over their life cycles in a regional context. Similar to other MFA tools, SFA focuses on input materials but furthermore follows substances within the economic system to trace outputs, wastes, and emissions. In practice, SFA is frequently used to trace persistent toxins, high-value recyclable materials, hazardous chemicals, or substances of regional concern. Some of the most recent applications of SFA are: (i) phosphorus budgeting in the context of a city, particularly for wastewater management (Tangsubkul *et al.*, 2005); (ii) investigation of nitrogen and phosphorus flows in different industrial sectors (Antikainen *et al.*, 2004); and (iii) evaluation of waste management alternatives by combining SFA and LCA within a decision making tool such as ORWARE (Bjorklund *et al.*, 1999). The MFA methodology is closely related to the ecologic view of *urban metabolism* (see for example Kaye *et al.* (2006)), since they share the interest for observing how materials enter, exit, or are accumulated in a system. If MFA is coupled with energy balances it becomes a useful tool for the evaluation of socioeconomic metabolism capable of differentiating between energetically dependent and material dependent economies (Huang *et al.*, 2006).

The methodology of SFA is selected over LCA and Exergy Analysis for several reasons. First, in the case of LCA, to prevent increasing the uncertainty level of the analysis, so socio-ecological indicators, as explained in Section 1.3.2 are preferred over highly uncertain impact factors that convert material inventory into potential environmental harm. Exergy, on the other hand, is more difficult to communicate than mass and energy terms, and requires intensive work to convert all flow into exergy terms, which could be impractical if a large system is analyzed in detail. Moreover, part of the objectives of this dissertation is to establish a sustainability assessment framework that reflects on specific substances related to the challenges described in Section 1.1.1, for which SFA fits appropriately.

2.1.5 Systems Analysis

System Analysis (SA) is the label given to the general approach used for understanding complex interactions among processes within a system. In principle, LCA, Exergy Analysis, and SFA are also a kind of systems analysis, but with a more specific focus. In the context of sustainability assessment, studies such as those produced by Chen and Beck (1997), Hellström *et al.* (2000) and Balkema (2003) have studied the water sector, while works such as that presented by Hosier (1993) elaborates on the energy sector. Balkema (2003) used system analysis with a similar structure to LCA to examine the Domestic Water System. The first phase consisted of defining boundaries of the system and sustainability indicators. Inventory analysis was performed in the second phase, in which indicators are valued quantitatively or qualitatively. The last phase, optimization, aims to minimize undesirable factors while maximizing benefits through the implementation of an objective function. This tool is an analytical approach focused on the operational phase of a service with a change-oriented character. The SA method, when embedded in a model-based decision support framework, emerges as a powerful tool for technology screening and identification of promising alternatives towards sustainability, see for example Balkema *et al.* (2001).

Using also a systems analysis approach, Chen and Beck (1997) proposed a methodology for screening processes of wastewater treatment technologies. A quantitative screening analysis was performed for over 120 unit processes with three conditions as the criteria for strong sustainability: (i) wastewater infrastructure shall be economically sustainable, (ii) persistent pollutants should be absent from all the product streams of the wastewater infrastructure, and (iii) products should not introduce distortions to material cycles, i.e. nutrient cycles.

In this case steady-state transfer functions are assigned to each technology to simulate the process unit performance and cost associated. The parameters of these functions are random values distributed uniformly and independently within specified lower and upper bounds. Technological strands or candidate technology combinations are generated considering the level or stage of treatment, competent technologies available for each level, and combining rules. Following a set of constraints, e.g. suspended solid content in effluent, satisfactory strands will be identified. The relative frequency at which a given technology is found in a successful strand is defined as *probability of survival*. Characteristics such as performance, robustness (recall Balkema's (2003) functional indicator), costs, land use, odor emissions, and nutrient recovery are inserted in the screening process in the form of constraints. This preliminary screening method serves as a tool for identifying promising technologies that should be prioritized for testing and development.

2.1.6 Space and Time Boundaries

A great deal of discussion is still taking place in the sustainability analysis context with regard to the definition of practical, but at the same time comprehensive, system boundaries. It is recognized that larger boundaries will reduce the omission of possibly critical aspects of the system, and prevent sustainability issues from being transfered in space (Balkema *et al.*, 2002). Atmospheric emissions are the typical example of a local issue that can have consequences elsewhere. Including as many unit parts of the chain of processes rather than a single process increases the possibilities for exploring a larger variety of alternatives. The ISO 14040 series for LCA suggests following up mass and energy flows entering or leaving the system directly to the environment, i.e. beyond any human transformation (Suh *et al.*, 2004). Decisions on inclusion or exclusion of processes are usually a subjective practice, especially because sometimes the negligibility of excluded processes is uncertain thus compromising the overall conclusions of the study. A number of studies have used either mass, energy or environmental relevance as a criterion to decide which inputs are relevant; however, the subjectivity of the environmental aspect and the lack of empirical basis — to establish for instance the proportionality between mass or energy and environmental consequences. A system boundary selection methodology was proposed by Raynolds *et al.* (2000) specifically for LCA studies of energy systems and called the Relative Mass-Energy-Economic (RMEE). A ratio is calculated by comparing each input and the system's functional unit on a mass, energy and economic basis. The practitioner selects a *cut-off* ratio value as an exclusion criterion. Again, there is no scientific basis to demonstrate that this method is enough to guaranteed a comprehensive approach (Suh *et al.*, 2004).

If complying with the recommendation of the ISO 14040 series is not possible, the integrated hybrid analysis model proposed by Suh *et al.* (2004) could be an alternative. It consists of the combination of two approaches: process analysis and economic input-output analysis (IOA). The first is based on a process flow diagram approach while the second relies on monetary transactions matrices among industry or economic sectors to describe complex interdependencies — usually within a national context. It is typical to use the process-based approach to represent the unit operations part of the core system, while IOA incorporates the surrounding economy to avoid truncation of far upstream or downstream processes. Suh *et al.* (2004) reported a difference of 18% between a hybrid analysis and a truncated, only process-based LCA, but it is recognized that this method involves a degree of uncertainty due to the large degree of aggregation of products and commodities and the fact that input-output data are usually outdated. However, the boundary selection between the process system and the IO system is still arbitrary and highly dependent on data availability.

Ideally, the best time scale of a sustainability study is to consider the whole life-cycle of the service or product, but this is usually accompanied by the requirement for vast amounts of data, for which reason most LCA studies include only the operation of the system. Subject to the quality of the data, more data could result in even more uncertainty than using better data and reducing the time frame of the study. It is therefore important to recognize the relevance of the life-cycle stages of the system. For instance, urban water systems have long operative life spans, typically about 20–50 years, making the operating stage the most relevant (Beck and Cummings, 1996). Intrinsically, the notion of sustainability is associated with long-term periods, especially when referring to the of human race, but the ultimate criteria is to define the scope of the study based on its objectives. (Lundin *et al.*, 2000).

2.2 Eco-efficiency and Eco-effectiveness

Simple sustainability metrics can be easily used by companies to assess their processes. Schwarz *et al.* (2002) proposed a set of five basic indicators upon which additional or more specific indicators can be developed. These indicators are:

- Material intensity
- Energy intensity
- Water consumption
- Toxic emissions
- Pollutant emissions

If two processes are compared based on these metrics, there must be an anchor point. In most cases, this anchor point is related to the output or purpose of the process, e.g. one metric tonne (t) of product. Thus, a better process would the one that generates more product per unit of resources used, that is, less *material intensity.* In other words, we are assessing the system in terms of its efficiency, which in many occasions, with a more specific purpose, is called *eco-efficiency.* Although *eco-efficiency* has been defined in many ways, in essence it means *producing more with less*, where *less* refers to resources and emissions (Côté *et al.*, 2006). However, those improvements reached by implementing eco-efficiency seem to vanish, particularly at a larger scale, e.g. national or global. Hofstetter *et al.* (2006) discusses, apart the obvious effects of population growth and economic development, two possible reasons:

(i) confounding effects due to extra efficiency achieved in using capital and labor, and (ii) the phenomenon of *psychological and physical rebound*. The latter includes market and social changes that will result in an increased use of the service or product. For example, efficiency is capable of reducing production cost which is reflected in lower consumer prices. Similarly, a service has reduced its environmental impact and its new benefits are publicly announced. In both cases the result could be an increase in consumption, and possibly, and increase in environmental harm.

McDonough and Braungart (2002) divide global metabolisms or cycles into the biological and the technological. The first refers to the nutrients useful for the biosphere (e.g. food, detergents, fabrics, cosmetics, shoe soles, and tires), while the technological is related to the materials required for industrial processes within the technosphere (e.g. computers, appliances, and materially stable parts of automobiles). The two in principle should be kept separated given that cross contamination diminishes the health, value, and effectiveness of either cycle. The mixing of these cycles promotes the generation of products that McDonough and Braungart call "monstrous hybrids". These kind of products are part of the daily life of everyone, and some of those products are sold as "environmentally friendly", but the reality is that separating and recovering the biological nutrients and technological materials constituting such products is nearly impossible, securing a future as a second class material after a process of "downcycling". An example of this, described by McDonough and Braungart, is the use of a mix of cotton and polyethylene terephthalate (PET) as an upholstery fabric. Cotton is seen as a natural product and PET was obtained from recycled plastic bottles making this product a good candidate for a positive environmental label. But if the health issues that can arise from the inhalation of abraded particles form the fabric and the difficulties to recover a good quality cotton from it are taken into account, the conclusion would be that the product is not really a sustainable one.

The term *eco-effectiveness* is embedded in the concept of *cradle-to-cradle* (C2C) introduced by McDonough and Braungart (2002). The C2C philosophy, based on the life-cycle of a tree, is expressed in three tenets:

(a) waste equals food — metabolisms are continuously regenerating.

(b) use solar input — solar energy is the only source that provides positive entropy, and

(c) celebrate diversity — human systems fit natural systems.

These tenets inspired the formulation of a set of twelve principles for green engineering design as described by McDonough *et al.* (2003) and Anastas and Zimmerman (2003),

Principle 1: Material and energy flows involved in the process or system should be inherently non-hazardous.

Principle 2: Preventing waste (non-usable product) formation is better than cleaning and remediation.

Principle 3: The designer of a process or system should prefer 'reversible' mixing of flows to ensure proper recovery, reuse, recycling, and beneficial disposal.

Principle 4: Implement efficient use of mass, energy, space, and time to prevent wasting of resources.

Principle 5: Avoid designing under a "one-size-fits-all" philosophy, which normally facilitates designing and construction, but often leads to unnecessary resources usage during operation.

Principle 6: Integrate material and energy flows within a unit operation, process, manufacturing facility, industrial park, or locality, to reduce raw material requirements.

Principle 7: Processes and systems should be designed, operated, and managed to be output-pulled rather than input-pushed (produce the amount needed).

Principle 8: Output Flows should be up-front engineered so that after their service life, commercial 'afterlife', they can not only be safely 'metabolized' within one of the nutrient cycles, i.e. biological or technological, but also provide adequate nourishment to it.

Principle 9: Design processes and systems so that output flows can be re-inserted in the corresponding nutrient cycle in a timely manner.

Principle 10: Complexity and entropy content should be taken into account when deciding recovery, reuse, recycle, and beneficial disposal paths.

Principle 11: Reducing the complexity of a flow, e.g. by adding functionalities to a material, facilitates its recovery, reuse, recycle, or beneficial disposal.

Principle 12: Renewing (or regenerating) rather than depleting: closing the cycles.

Although these principles are still in a more or less conceptual form, they offer a first illustration of how to put into practice the three tenets described above. The principles can be generally classified into safety and health (principle 1), efficiency (principles 2 to 7), and effectiveness (principles 8 to 12). The latter group is arguably associated with the health of the nutrient cycles. From the analysis presented in this section, it is clear that if a system or product is built inherently *good* then the solution is independent of market and social changes, thus sustainable. A system that complies with the principles of eco-effectiveness has increased chances to generate *spare resource capacity*, which from the view point of Wilkinson and Cary (2002) is an important component of resilience of production systems and sustainability.

2.3 Nutrient Cycles

The present section is a summary of nutrient cycles in natural and human-managed systems, with a focus on large-scale processes, such as leaching, runoff, deposition, denitrification, volatilization, photosynthesis, and respiration, rather than examining nutrient cycles at the microbial level. The purpose is to identify the main drivers of these processes and draw differences between rural and urban areas.

2.3.1 The Nitrogen Cycle

Nitrogen is the most abundant element in the atmosphere and one of the most studied substances given its involvement in almost every aspect of nature and human life. A general scheme is presented in Figure 2.2 that includes mainly soil processes and their relevance to nitrogen export fluxes. The magnitude of nitrogen transported depends on numerous aspects, besides the obvious hydrological controllers (e.g. soil morphology, slope, vegetation, and precipitation), such as nitrogen availability — a function of the amount of N applied to land and how much of this is labile, volatilization, microbial activity, and plant uptake. Nitrogen can be found in soluble or gaseous form. The latter is typically reported as elemental N or diatomic N (N_2). On many occasions nitrogen concentration in soluble form is reported as Total Kjehldahl Nitrogen (TKN) which refers to the sum of total organically bound nitrogen (TON), ammonia (NH_3-N), and ammonium (NH_4-N). Total nitrogen (TN) is calculated as TKN plus the concentration of nitrate-N (NO_3-N) and nitrite-N (NO_2-N). Total Inorganic Nitrogen (TIN) is then the sum NH_4+NO_3+NO_2.

Food production relies heavily on synthetic fertilizers, as a source of nitrogen, supplied in different forms: anhydrous ammonia NH_3, urea $(NH_2) \cdot 2CO$, ammonium sulfate $(NH_4) \cdot 2SO_4$, and ammonium nitrate $NH_4 \cdot 4NO_3$. Current levels of food and timber production would not be possible without fertilization. For example, a one-time application over a six-year period of 168 to 224 kg N ha^{-1} plus 28 kg P ha^{-1} provides a growth gain of 30% compared

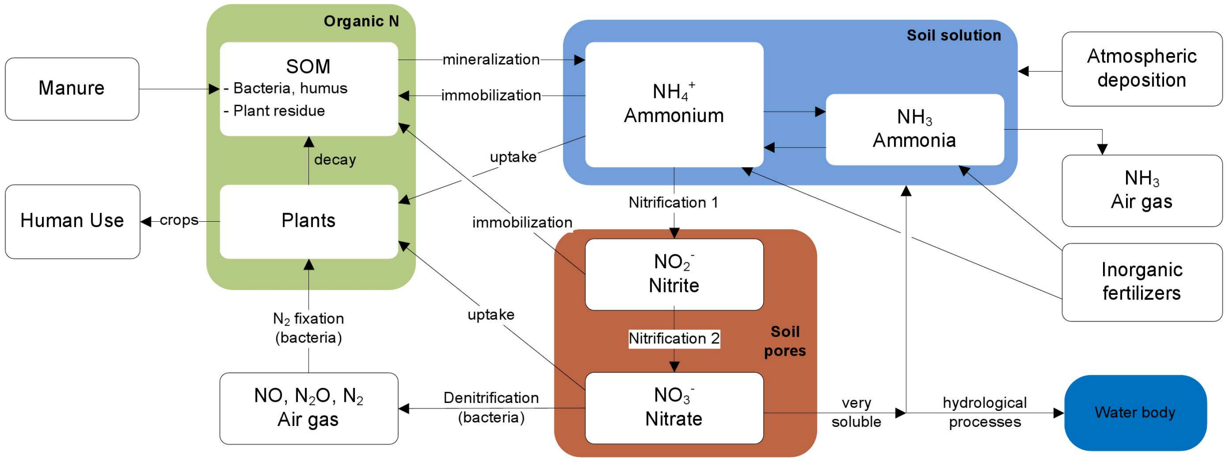

Figure 2.2: General scheme of the soil nitrogen cycle and associated export processes.

to no fertilizer (Fox *et al.*, 2006). It has been found that about 39–68% of the fertilizer N is recovered by crops, and less than 10% is lost via leaching (Dowdell and Mian, 1982). The rest is lost via runoff or volatilized. Fertilizer application rate and the time of application with respect to rainfall occurrence are significant in the process of nitrogen percolation through the root zone (Hower *et al.*, 2005; Kirchmann, 1994). Leaching typically occurs in the form of nitrates (NO_3), representing from 63% (Harriman, 1978) to almost 100% of the total nitrogen concentration in leachate (Dowdell and Mian, 1982). However, fertilization with organic manures can lead to leaching of dissolved organic nitrogen or DON (Kirchmann, 1994), although Currie *et al.* (1996) found that DON variability is less dependent on the fertilization rate compared with Dissolved Inorganic Nitrogen (DIN), thus the type of fertilizer used has also an impact on the leaching process. Moreover, nitrogen leaching from animal manure might be higher in the long term, i.e., more than 3 years, compared to inorganic fertilizer (Bergstrom and Kirchmann, 1999). Similarly, controlled-release fertilizers have shown reduced losses of in simulated grass surfaces compared with balanced soluble forms (Shuman, 2001). Nitrogen percolation can be estimated by the empirical Equation (2.1) originally designed by Simmelsgaard (1998) and tested also by Hansen *et al.* (2000),

$$N_{leaching} = e^{(1.136-0.06628\cdot clay+0.00565\cdot N_{applied}+Crop)} \cdot d^{0.416} \tag{2.1}$$

where $N_{leaching}$ is the nitrogen leached in $\mathrm{kg\,ha^{-1}}$ per year, *clay* is the percentage of clay in the upper 0–25 cm of the soil, $N_{applied}$ is the nitrogen applied to the soil in $\mathrm{kg\,ha^{-1}}$ per year, *crop* is the type of crop, and d is the water percolated into soil in $\mathrm{mm\,y^{-1}}$. Leaching is a process that is mainly controlled by soil properties, nitrogen input to the soil through fertilization and plant decay, and percolated water from precipitation. Table 2.4 presents a summary of concentrations of N in leaching under different land management strategies.

Dry and wet deposition is also a relevant process. In natural ecosystems, this a major source of N besides the N fixation ability that some plants and bacteria have to collect atmospheric nitrogen, while in the case of Phosphorus (P), deposition and erosion of watershed soils are the only input for plants. There are numerous sources for airborne nutrients, but wind erosion, oceanic aerosols, bird droppings are possibly the most important components in natural systems. However, combustion of fossil fuels, waste incineration, and soil tillage have become increasingly relevant (Ahn and James, 2001; Anderson and Downing, 2006). In estuaries, deposition can account for 10–40% of new N entering the system (Gao *et al.*, 2007). Table 2.5 compiles values obtained in previous studies as a reference for the magnitude of the deposition process for nitrogen and phosphorus. By comparing the values of nitrogen leaching from forests (take for example NO_3) and the input from precipitation, one can conclude that deposition is a relevant component for systems with minimum human intervention.

Surface runoff is a particularly important process for the transport of nutrients from land to streams in the form of diffuse sources. Similar to other hydrological processes, runoff

Table 2.4: Concentration in leachate and leaching rate of nitrogen from soils under different land management strategies.

Land Use	**Management Strategy**	**Nitrogen Leaching**[a]	**Reference**
Forest	undisturbed, unfertilized	0.05–0.15 NO_3-N	(Kubin, 1998)
	clear cut, ploughed,	0.10–0.60 NO_3-N	(Kubin, 1998)
	undisturbed, unfertilized	0.5–1.0 DON-N	(Piirainen *et al.*, 2007)
	undisturbed, unfertilized	0.1–0.3 NO_3-N	(Piirainen *et al.*, 2007)
	undisturbed, unfertilized	0.1–0.8 NH_4-N	(Piirainen *et al.*, 2007)
	clear cut, harrowed	0.6–2.0 DON-N	(Piirainen *et al.*, 2007)
	clear cut, harrowed	0.1–0.4 NO_3-N	(Piirainen *et al.*, 2007)
	clear cut, harrowed	0.8–2.0 NH_4-N	(Piirainen *et al.*, 2007)
	unfertilized	0.03 DIN[b]	(Aber *et al.*, 1998)
	unfertilized	0.54 DON[b]	(Aber *et al.*, 1998)
	inorganic fertilizer applied	0.21 DIN[b]	(Aber *et al.*, 1998)
	inorganic fertilizer applied	0.36 DON[b]	(Aber *et al.*, 1998)
Grass	fertilized	11–20 TN[b]	(Hansen *et al.*, 2000)
Crops	pigs farms, varied crops	3.0–11 TN[b]	(Hansen *et al.*, 2000)
	manure fertilizer	5.7 NO_3-N[b]	(Basso and Ritchie, 2005)
	compost or Urea	3.4 NO_3-N[b]	(Basso and Ritchie, 2005)
	no fertilizer added	2.6 NO_3-N[b]	(Basso and Ritchie, 2005)

[a] See Appendix A for chemical symbols and abbreviations. Unless otherwise noted units are in $mg\,l^{-1}$.
[b] Leaching rate $g\,m^{-2}\,y^{-1}$.

Table 2.5: Example of values for atmospheric dry and wet deposition of nitrogen and phosphorus for different regions.[a]

	Deposition		**Remarks**	**Source**
	Dry $\mu g\,m^{-2}d^{-2}$	**Wet** $mg\,l^{-1}$		
TN	530–810	0.15–1.4	Agricultural area, Ohio	(Anderson and Downing, 2006)
		0.12–0.24	Data for Connecticut	(Nadim *et al.*, 2003)
	0.8–4.0[c]	3.5–7.0[c]	Rural areas in Canada	(Zhang *et al.*, 2009a)
	2.1[c]	4.2[c]	Data for Metro Atlanta	(Peters *et al.*, 2002)
	14[c]		Forest in NE Australia	(Puxbaum and Gregori, 1998)
NO_x-N	350–470	0.1–0.8	Agricultural area, Ohio	(Anderson and Downing, 2006)
		1.0–1.5	Georgia State region	(EPA, 1999)
	30–45[b]	3.7–5.4[b]	New Jersey coastal area	(Gao *et al.*, 2007)
		9.7–60[e]	Seoul, South Korea	(Park and Lee, 2002)
	380	0.53	Ontario, Canada	(Ro *et al.*, 1988)
NH_x-N	60–88	0.02–1.5	Agricultural area, Ohio	(Anderson and Downing, 2006)
	19–25[b]	1.7–7.8[b]	New Jersey coastal area	(Gao *et al.*, 2007)
		20–114[e]	Seoul, South Korea	(Park and Lee, 2002)
		1.5–2.0	Georgia State region	(EPA, 1999)
TP	82	9.4[d]	Florida everglades	(Ahn and James, 2001)
	84–104	4.0–25[d]	Agricultural area, Ohio	(Anderson and Downing, 2006)
SRP	34–44	0.4–4.0[d]	Agricultural area, Ohio	(Anderson and Downing, 2006)
	11	17[f]	Lake Huron, Michigan	(Delumyea and Petel, 1978)

[a] See Appendix A for chemical symbols and abbreviations.
[b] Units of concentration $mmol\,m^{-2}\,y^{-1}$.
[c] Deposition rate units $kg\,ha^{-1}\,y^{-1}$.
[d] Units of concentration $\mu g\,l^{-1}$.
[e] Units of concentration $mol\,l^{-1}$.
[f] Deposition rate units $\mu g\,m^{-2}\,d^{-2}$.

contribution to stream nutrient concentration depends to a great extent on land management practices. Table 2.6 shows how different fertilization techniques affect the concentration of nutrient in surface runoff. Losses of nutrients have been also calculated through the use of empirical export coefficients, estimated for each land use (Johnes, 1996). Equation (2.2) shows the mathematical expression of the nutrient export model,

$$R_{losses} = E_c \cdot \mathrm{A} \cdot N_{input} + N_p \tag{2.2}$$

where R_{losses} is the nutrient loss from the soil via surface runoff in kg ha^{-1}; E_c is the export coefficient as a percentage; A is the area associated to the losses in hectares; N_{input} is the nutrient input to the soil in kg ha^{-1}; N_p is the nutrient contribution of precipitation. Typical values for woodland (no fertilizer added) are 13 kg ha^{-1} and 0.02 kg ha^{-1} for N and P respectively. Relative to the inputs, the losses of N from grassland, cereal crop, and row crops are 5, 12, and 20% respectively, while estimated losses of P from grassland, cereal crop, and row crops vary from 1.5 to 3% (Johnes, 1996).

Table 2.6: Typical values of surface runoff of total nitrogen (TN) and total phosphorus (TP) from cropland under different management strategies.

Management	**Runoff composition**		**Reference**
Strategy	**Nitrogen**	**Phosphorus**	
Agricultural plots, swine manure	–	10–14.3	(Gessel *et al.*, 2004)
Pasture plots, no fertilizer	1.1	0.28	(Mc Leod and Hegg, 1984)
Pasture plots, NH_4+NO_3	7.5–57	1.8–4.2	(Mc Leod and Hegg, 1984)
Pasture plots, dairy manure	8.0–20	5.0–8.0	(Mc Leod and Hegg, 1984)
Pasture plots, poultry manure	9.0–43	3.0–12	(Mc Leod and Hegg, 1984)
Pasture plots, municipal sludge	5.0–10	2.0–4.2	(Mc Leod and Hegg, 1984)

In natural ecosystems, there are two processes that return the nitrogen captured from the atmosphere: denitrification and volatilization. The first is mostly a biological process promoted by bacterial activity that releases N_2 and, in less quantities, N_2O. The ratio N_2:N_2O depends on how well the field is drained, typically being 16, but some studies have shown N_2:N_2O=32. As in any process carried out by microbial activity, the main drivers are temperature, moisture, and availability of food (carbon). In cropland, it has been found that the type and amount of fertilizer applied together with irrigation has a strong influence over denitrification (Sánchez *et al.*, 2001; Dowdell and Mian, 1982), meaning that land use and management strategies can be a determining aspect to characteristics of the process. In forests, almost 70% of the denitrification process takes place within the upper soil layer, 0–10 cm, and it is in the same forest floor where nitrification occurs to account for about 75% of all the nitrogen input to forest watersheds (Todd *et al.*, 1975). Volatilization on the other hand, is a release mostly in the form of ammonia NH_3 and nitrogen oxides NO_x gas from organic and inorganic sources, e.g. fertilizers, manure, decaying plant material, as a function of moisture and temperature. Volatilization does not only take place in land application, but also during manure handling and storage. Losses, estimated as the difference between fresh manure and land applied manure, are 35% for poultry litter, 25% for anaerobic pits, 60% oxidation ditches, and 80% for lagoons, with the last three practices relevant for cattle and swine manure handling (Risse, 2009). Nitrogen volatilization, as NH_3+NO_x, from fertilization is typically in the range of 3.0–30% for inorganic fertilizer and 5.0–50% for organic sources of nutrient (IPCC, 2006a).

2.3.2 The Phosphorus Cycle

The earth's crust is a main pool for phosphorus, reaching streams by weathering and erosion, to later be discharged into oceans. In order to return to land, ocean plates need to be exposed meaning that the natural phosphorus cycle is extremely long from the human perspective, thus cataloged as a non-renewable resource. Phosphorus fertilizer is usually obtained by mining phosphate rock in forms such as fluoro-apatite ($3Ca_3(PO_4)_2 \cdot CaF_2$), chloro-apaptite ($3Ca_3(PO_4)_2 \cdot CaCl_2$), and hydroxy-apatite ($3Ca_3(PO_4)_2 \cdot Ca(OH)_2$). Similarly to N, phosphorus is an essential nutrient for plants and animals, and therefore has a normal circulation through plants, soils, and hydrological paths, but it differs significantly at the same time because P does not have a significant gas phase component. Once phosphorus is made available for plants it is incorporated as organic phosphorus in the form of Deoxyribonucleic acid (DNA), Ribonucleic acid (RNA), and Adenosine triphosphate (ATP). Figure 2.3 shows the interaction between soil processes and export mechanisms of P, namely runoff, interflow, and leaching, operating in a similar way as explained for nitrogen. P is transported mostly as orthophosphates (PO_4-P) and in sediment-bound phosphorus released due to erosion.

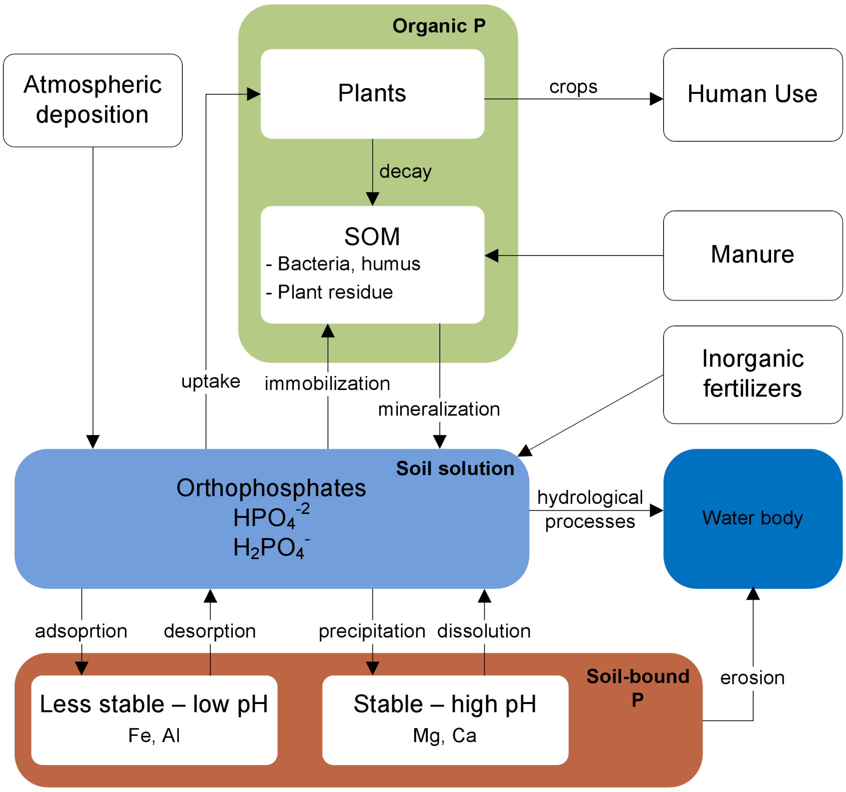

Figure 2.3: General scheme of the soil phosphorus cycle and associated export processes.

In one year, phosphorus losses in surface runoff can account for about 5% of the fertilizer applied in forested watersheds (Harriman, 1978), while unfertilized forests can show losses in the range between 0.1–0.15 $kg\,ha^{-1}$. However, forests still exhibit a phosphorus retention behavior given that the input through rainfall can exceed losses via drainage by three fold without any fertilizer applied (Harriman, 1978). Other studies, at a plot level, have shown no substantial difference between the runoff events from plots treated with different fertilization techniques. Nutrient concentration was more sensitive to the time between the fertilizer application and the precipitation event (Smith *et al.*, 2009).

Total phosphorus in soil leaching has been found to be around 2–8% of the fertilizer applied (Godlinski *et al.*, 2004). In the case of unfertilized forests, leaching is proportional, about 4%, to the P content in the organic layers in the forest floor. It happens similarly for N with a ratio near 6% (Cortina *et al.*, 1995).

Table 2.7: Concentration in leachate and leaching rate of phosphorus from soils under different land management strategies.

Land Use	**Management Strategy**	**Phosphorus leaching ($mg\,l^{-1}$)[a]**	**Reference**
Forest	undisturbed, unfertilized	0.1–0.5 PO_4-P	(Piirainen *et al.*, 2007)
	clear cut, harrowed	0.2–0.8 PO_4-P	(Piirainen *et al.*, 2007)
Grass	fertilized sandy loam	0.01–0.10 TP	(Godlinski *et al.*, 2004)
Crops	fertilized sandy loam	0.01–0.07 TP	(Godlinski *et al.*, 2004)

[a] See Appendix A for chemical symbols and abbreviations.

Sources of phosphorus available for deposition are mainly soil erosion and combustion of fuels. About 1.0% of the phosphorus in coal is released as airborne particles, while for municipal solid waste (MSW) incineration is about 0.6% (Mahowald *et al.*, 2008). Total phosphorus input to land from atmosphere deposition, wet and dry, is typically in the range 10–40 $kg\,P\,km^{-2}\,y^{-1}$ (Jennings *et al.*, 2003). Total phosphorus concentration in precipitation, wet deposition, can reach values of $9.4 \times 10^{-3}\,mg\,P\,l^{-1}$ (Ahn and James, 2001). The same study reported an average total P load of $112 \times 10^{-3}\,\mathrm{mg\,P\,m^{-2}\,d^{-1}}$, with a dry to wet ratio of 2.8 in mass terms.

2.3.3 The Carbon Cycle

Based on the description of the global carbon cycle by Schlesinger (1997), natural processes are the largest components. The major pools of carbon are the ocean, soils, atmosphere, and vegetation, sorted from largest to smallest. The total net flux to the atmosphere of $6.9\,\mathrm{Gt\,C\,y^{-1}}$ is observed, of which $6.0\,\mathrm{Gt\,C\,y^{-1}}$ is the sum of fossil fuels burning and $0.9\,\mathrm{Gt\,C\,y^{-1}}$ net vegetation destruction, associated with changes in land use too. Of the total net flux, $2.0\,\mathrm{Gt\,C\,y^{-1}}$ are dissolved in the ocean and $3.2\,\mathrm{Gt\,C\,y^{-1}}$ are being accumulated in the atmosphere, while the remaining $1.7\,\mathrm{Gt\,C\,y^{-1}}$ has an unknown fate. Annual carbon releases from fossil fuels represent only 0.8% of the total amount in the atmosphere, but when compared with the carbon accumulation rate the in atmosphere, it represents 53%, while the rest is accumulated in natural sinks, i.e. the ocean and land. However, these figures correspond to years prior to 2000, and the estimates for 2010 are 30% higher, up to about $9.0\,\mathrm{Gt\,C\,y^{-1}}$. Cities are a big driver, accounting for 71% of global enery-related CO_2 emissions (Canadell *et al.*, 2009).

At a smaller scale, land keeps playing an important role in the carbon cycle, as depicted in Figure 2.4. Carbon is originally incorporated into plant organic matter as part of the photosynthesis process, but then partially released as CO_2 due to plant decay. The rest is immobilized by soil microbes and later incorporated into the soil organic matter as CO_2 continues to be produced as the result of heterotrophic respiration. The labile portion of the soil carbon pool, together with mineralized sources of carbon, are then available for transport by hydrological processes in the form of Dissolved Organic Carbon (DOC) and Dissolved Inorganic Carbon (DIC) respectively. Although the global C cycle is dominated by photosynthesis and respiration, the flow of carbon in aquatic streams, 1.9 Gt per year, is not irrelevant (Öquist *et al.*, 2009). On the basis of the C cycle description above, the aquatic flux of C is over 30% of the flux derived from fuel combustion. Organic carbon from upland cool temperate watersheds in the US can be exported at a rate of 15–150 kg ha^{-1} y^{-1} (Mulholland and Kuenzler, 1979). However, studies carried out in rural environments, have found that carbon in water bodies is not as variable as N and P. A study carried out for four years on seven small catchments found that Total Organic Carbon (TOC) concentration in runoff remained more or less constant at 11 mg l^{-1}, revealing that the mineral origins of carbon can be significant to river carbon concentration (Haaland and Mulder, 2010). Moreover, perennial springs have been found responsible for the presence of some minerals, carbon, and other solutes in streams, contrary to N and P which are highly influenced by instream processes (Mulholland, 1992). The major human-related source of carbon for streams and lakes are runoff from manure land applications — releasing organic carbon, sewage discharges, and urban runoff. The latter can reach 500 mg l^{-1} in terms of chemical oxygen demand (COD) (Choe *et al.*, 2002). The concentration of carbon in leaching originates mostly in surficial zones of the soil, from humified SOM, and then "filtered" to a certain extent as it flows downwards by microbial utilization or stabilization in mineral-bound organic matter (Sanderman *et al.*, 2008).

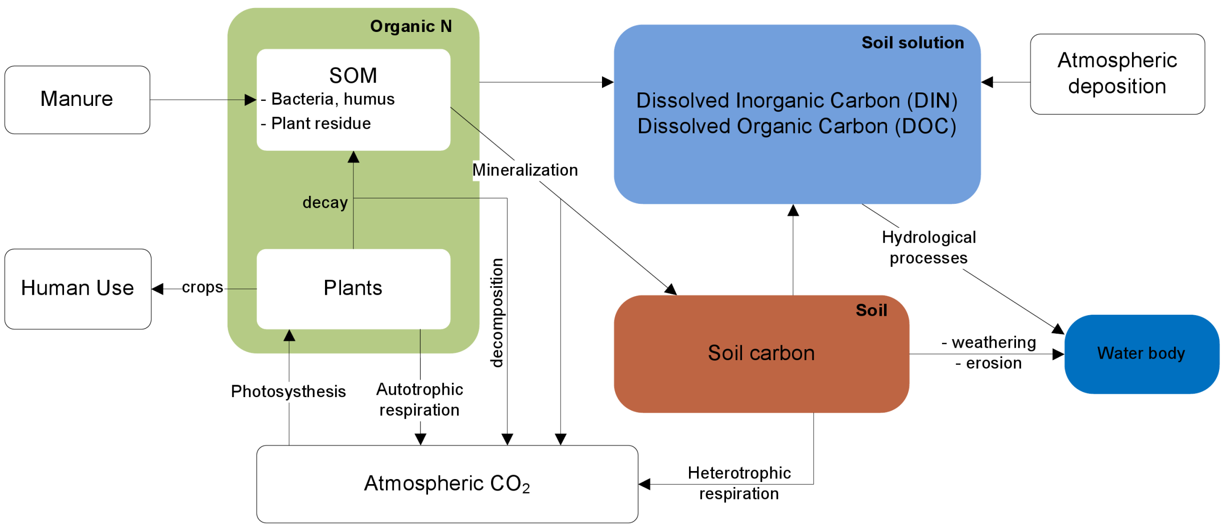

Figure 2.4: General scheme of the soil carbon cycle and associated export processes.

Table 2.8: Typical fluxes of carbon in leachate, runoff, and deposition.

Process	**Land use**	**Rate or composition**[a]	**Reference**
Deposition	California (wet)	2.0–18.6 TOC	(Kawamura *et al.*, 2001)
	Arizona (dry)	0.2–1.2 OC[b]	(Lohse *et al.*, 2008)
Leachate	undisturbed forest	30–40 DOC	(Piirainen *et al.*, 2007)
	disturbed forest	40–80 DOC	(Piirainen *et al.*, 2007)
Runoff	undisturbed forest	40–50 TOC	(Åström *et al.*, 2005)
	unfertilized forest	2.0–15 TOC	(Haaland and Mulder, 2010)
	coastal prairie	5.0–20 DOC	(Sanderman *et al.*, 2008)
	fertilized forage	2.0–32 DOC	(Sanderman *et al.*, 2008)
	agricultural area	3.6–7.9 TOC	(Cronan *et al.*, 1999)

[a] See Appendix A for chemical symbols and abbreviations. Unless otherwise noted units are in $\mathrm{mg\,l^{-1}}$.
[b] Dry deposition rate $\mathrm{g\,m^{-2}\,y^{-1}}$.

Carbon also enters the land in the form of wet and dry deposition, see Table 2.8. Values of Dissolved Organic Carbon (DOC) in the order of 7.4–9.4 kg/ha have been found for wet deposition, in precipitation (Piirainen *et al.*, 2002). Pure water has a neutral pH of 7.0. Normal rain is slightly acidic because of the carbon dioxide dissolved in rain water, so that normal pH is expected to be about 5.5, but near urban areas pH might be lower, mostly due to the increased presence of SO_2 and NO_x gases. For example, the metro Atlanta area exhibits an annual average of about pH 4.5–4.7 (sampling site GA41 of the US National Atmospheric Deposition Program).

2.3.4 Anthropogenic Disturbances of Nutrient Cycles

Land application of manure and fertilizer is responsible for the emission of ammonia (NH_3), a gas known for its adverse effects on human and animal health. Fossil fuels contain nitrogen that after combustion is released in the form of nitrogen oxides (NO_x) and other N chemical forms. Nitrous Oxide (N_2O) is a powerful greenhouse gas, important in climate change, and an ozone-depleting substance. It is produced by both natural, mainly microbial action in forests, and human-related sources such as agricultural soils, manure handling, and combustion. Depending on the nitrogen species, between 40 and 80% of global nitrogen emissions are related to human activities. The N transfer from atmosphere to biologically available pools, currently 100–150 $\mathrm{Gt\,N\,y^{-1}}$, has doubled in part due to fertilizer production ($\approx$80 $\mathrm{Gt\,N\,y^{-1}}$). This increment of N availability at the land level has implications over the global C cycle and the explanation of the missing sink of 1.7 $\mathrm{Gt\,C\,y^{-1}}$ (Vitousek *et al.*, 1997).

In streams, N and P are essential elements for plant and algae growth, but high concentrations bring potential issues for human and ecosystem health. For example, NO_3-N concentrations can have serious toxicological and ecological effects. The US Environmental Protection Agency USEPA)has established a maximum of 10 $\mathrm{mg\,l^{-1}}$ in drinking water to prevent methemoglobinemia, a potentially fatal disease affecting primarily infants. Although concentration levels rarely exceed the threshold proposed by USEPA, agricultural areas handling livestock and under intensive fertilization regimes can easily exhibit higer values (Smith *et al.*, 1993). Eutrophication is a natural process in the aging of lakes and some estuaries, but excess of N and P is a concern with regard to levels of eutrophication that interfere with designated uses of aquatic bodies and the health and diversity of indigenous fish, plant, and animal populations. Although P is typically the limiting nutrient controlling the rate of eutrophication, N has been found responsible for the increased presence of algae in coastal areas (Howarth and Paerl, 2008). Human activities, e.g., wastewater treatment effluent and agricultural run-off, can make phosphorus available in larger quantities, accelerating algae and other aquatic plants growth, particularly in lakes and estuaries. Increased aquatic vegetation depletes dissolved oxygen, can lead to undesirable tastes, color, and odors in the water. EPA recommends an upper limit of $0.1\,\mathrm{mg\,l^{-1}}$ as the standard for total phosphorus (TP) in streams (Smith *et al.*, 1993). The banning of phosphorus-based detergents in the 1970's decreased significantly the discharge of phosphorus to receiving water resulting in the improvement of numerous ecosystems (Maki *et al.*, 1984). However, P and N runoff from agricultural land, as non-point sources of nutrient discharges, remains a major challenge (Dougherty *et al.*, 2004; Sharpley *et al.*, 2006). Surface runoff from urban areas provides nutrients to streams with concentrations comparable to the values reported for agricultural land, see Table 2.9 and 2.6, but given that more precipitation over impervious areas is available as runoff, its contribution should not be ignored.

Table 2.9: Average concentration of nitrogen, phosphorus, and carbon in urban runoff in South Korea(Choe *et al.*, 2002).[a]

	Concentration ($\mathrm{mg\,l^{-1}}$)	
	Residential	Industrial
TKN	8.5	5.1
TP	2.0	1.9
COD	313	80

[a] See Appendix A for chemical symbols and abbreviations.

2.4 Uncertainty Management

Within the environmental modeling context, sources of uncertainty can be classified under three categories: *structural*, *parametric*, and *circumstantial*. The first refers to the representation, in the form of mathematical expressions, of the conceptual image — the structure — of the system; the second is about the parameters that control the behavior of the model as defined by its structure; the third refers to the uncertainty associated with model inputs, such as initial conditions, calibration data, and forcing functions (Beck, 1987, 1991). The conglomerate of hypotheses constituting the conceptual image are often incapable of reproducing the complex interaction of internal processes of environmental systems (Osidele and Beck, 2001). Model structure is based on usually limited knowledge of the system and its behavior, thus structural uncertainties are frequently ignored. Monte Carlo simulation has been used in the past to account for data inaccuracy in Life Cycle Inventories (Huijbregts *et al.*, 2001). Regionalized Sensitivity Analysis (RSA), a more specific procedure, but also based on Monte Carlo simulation, has been successfully used for modeling agricultural watershed hydrology (Kim and Delleur, 1997), instream water quality (Osidele *et al.*, 2003; Arabi *et al.*, 2007), and water quality management programs (Lence and Takyi, 1992). The purpose of using RSA has been generally identifying (i) optimal combinations of parameter values, (ii) appropriate model structures, (iii) the reachability of community values, and (iv) *key* uncertainties in the model parametrization. Consequently, RSA, as opposed to an optimization routine, fits appropriately the objectives of this dissertation, because it is more informative about the behavior of the system (as described by the model) and rather than searching for the best set of parameter values, it accounts for the uncertainty of model parameters, which represents better the interaction of human systems with the environment. The RSA procedure involves several steps as follows,

(1) Parameters of interest are selected for uncertainty-sensitivity analysis.

(2) An operational range is defined for the parameters based on literature, laboratory tests, or expert knowledge.

(3) A vector of trial values of each parameter is generated. The Latin Hypercube Sampling (LHS) strategy is useful to achieve a uniform coverage of the parameter domain requiring fewer sampling trials (Osidele, 2001). Thus, it has been assumed that the parameter space has a uniform distribution.

(4) A criterion or set of criteria is defined to reflect the desirable behavior of the model output $\{B\}$, and whatever output value that falls outside the $\{B\}$ domain, is defined as the non-behavior $\{NB\}$.

(5) The model outputs obtained from the Monte Carlo simulation are segregated in a binary fashion as either $\{B\}$ or $\{NB\}$.

(6) Based on the previous step, it is possible to classify each element α_j, belonging to the parameter sample vector, into two groups: $\{\alpha_j|B\}$ and $\{\alpha_j|NB\}$. A marginal cumulative distribution is built for each group.

(7) The Kolmogorov-Smirnov (K-S) two-sample test (two-sided version) is performed at a significance level, to establish whether the parameter values corresponding to $\{\alpha_j|B\}$ and $\{\alpha_j|NB\}$ are part of the same population. The Statistical hypothesis is formally expressed as:

$$\begin{aligned} H_o : f_m(\alpha_j|B) &= f_n(\alpha_j|NB) \\ H_1 : f_m(\alpha_j|B) &\neq f_n(\alpha_j|NB) \\ \text{Test statistics: } d_{m,n}(\alpha_k) &= sup_x \,\|F_m(\alpha_j|B) - F_n(\alpha_j|NB)\| \end{aligned}$$

Where $F_m(\alpha_j|B)$ and $F_n(\alpha_j|NB)$ are the cumulative distributions corresponding to a number of m behaviors and n behaviors; $f_m(\alpha_j|B)$ and $f_n(\alpha_j|NB)$ are their respective probability density functions; sup_x refers to the x value at which the largest vertical difference between marginal cumulative distributions exists;

(8) A set of significance cutoff levels can be selected for rejecting the H_o hypothesis as a way to rank the importance of parameters.

(9) The values of $d_{m,n}$ are compared to the critical values of the Kolmogorov statistical distribution defined using the set of significance cutoff levels. Parameters are classified based on their level of importance. For instance, $\alpha = 0.05$ and $\alpha = 0.15$ for key and important

parameters respectively, while any parameter with a $d_{m,n}$ — that works inversely to the significance level — smaller than the statistical critical value corresponding to $\alpha = 0.15$ is deemed redundant.

Another aspect of the RSA procedure is the definition of the $\{B\}$. In order to obtain a statistically significant number of model behaviors $\{B\}$ and non-behaviors $\{NB\}$, the conditions selected cannot be too restrictive or too relaxed. This requires extensive knowledge of the model structure and its limitations, as well as understanding the desirable targets that stakeholders might have with respect the actual system that it is being modeled.

Building upon the concepts and methods described in the present chapter, the next Chapter 3 is devoted to explain how the methodologies selected fit together and how they are implemented to construct the Multi-Sectoral Analysis (MSA) framework.

Chapter 3

THE MULTI-SECTORAL SYSTEMS ANALYSIS FRAMEWORK

"Analysis has to be applied when we intend to thoroughly understand, determine or find out the facts, relationship or processes involving the dynamic nature of the constituents in any scientific matter or subject." P. Keshava Bhat

The objectives and approach for this dissertation declared in Chapter 1 were followed by the compilation of the knowledge, presented in Chapter 2, required to build a coherent framework for systems analysis of five industrial sectors. The purpose of this framework is evaluating the level of sustainability, in terms of socio-ecological flows, using a rather unconventional combination of methodologies and measures that are explained in the present chapter.

3.1 Methodological Framework

The methodology is structured as described in Figure 3.1. The Multi-sectoral model and both procedures, the Monte Carlo sampling — specifically the Latin Hypercube Sampling (LHS) method — and the Regionalized Sensitivity Analysis (RSA) are the core of the framework. Input data are fed to the computational framework and outputs are generated. This output offers the necessary information to carry out the analysis that leads to conclusions or recommendations for system improvement. All the procedures are coded in MATLAB®, but input and output data are available to the user and accessed via EXCEL®. Appendix B presents the list of parameters and inputs that are specified for the MSA. The model coding structure is presented graphically and described in Appendix C. The use of this framework has to follow a set of steps:

(i) Defining the objective and scope of the analysis to be carried out. This includes defining the boundaries of the system which should be preferably as ample as possible to increase the chances of success of the analysis, i.e. find key flows or processes for the improvement of the system towards sustainability.

(ii) Collecting specific data for the system based on its spatial boundaries and the scope of the analysis. The more system-specific data are used the better is represented the actual system by the model. These data must be added to the input file *MSAinput.xls*.

(iii) Simulating and analyzing output data. Because of the structure of the modeling framework, it is possible to run the simulation in two modes: only as a material and energy accounting exercise (no RSA) and as an identification tool for which elements of the model are *critical* (with RSA). In both cases, there is access to the information that the sustainability indicators, defined in Section 3.1.2, can provide about the performance of the system.

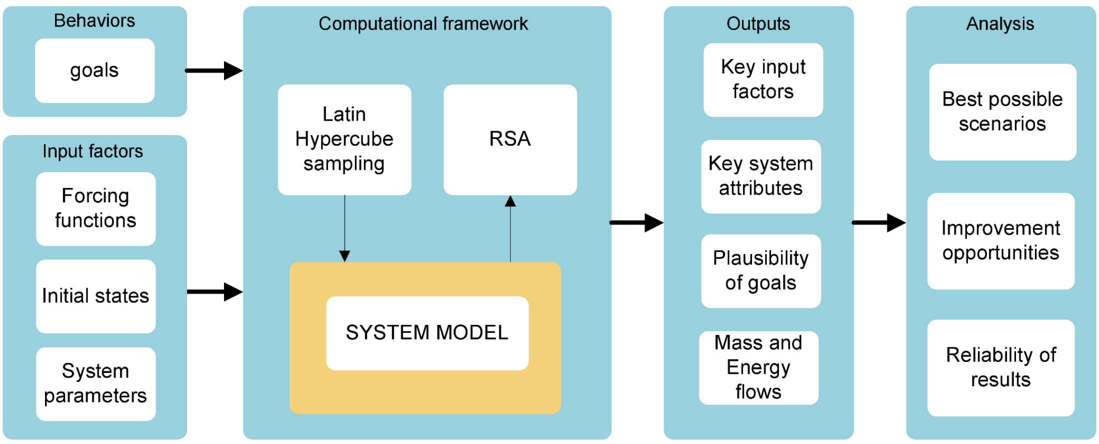

Figure 3.1: General scheme of the proposed computational framework of the MSA+RSA.

3.1.1 Structure of the Multi-sectoral model

The present work is focused on the flows of water, nutrients (N, P, and C), and energy. Therefore, the Substance Flow Analysis (SFA) proposed herein includes five technical sectors: water, energy, forestry, food, and waste management — hence Multi-sectoral — with emphasis on the operation phase. The Multi-sectoral model is capable of processing and generating information for one year of simulation; therefore, it is not a tool for transient analysis. A detailed flow diagram was developed for each sector to represent flows and unit processes of interest. Each unit process represents an activity within the system that involves the mixing, separation, or transformation of flows. Figure 3.2 shows a summarized version of the five sectors involved. Sectors are interconnected between each other by material and energy flows. Each sector has inputs and outputs from other sectors and the environment, this being represented by the hydrosphere, the lithosphere, and the atmosphere.

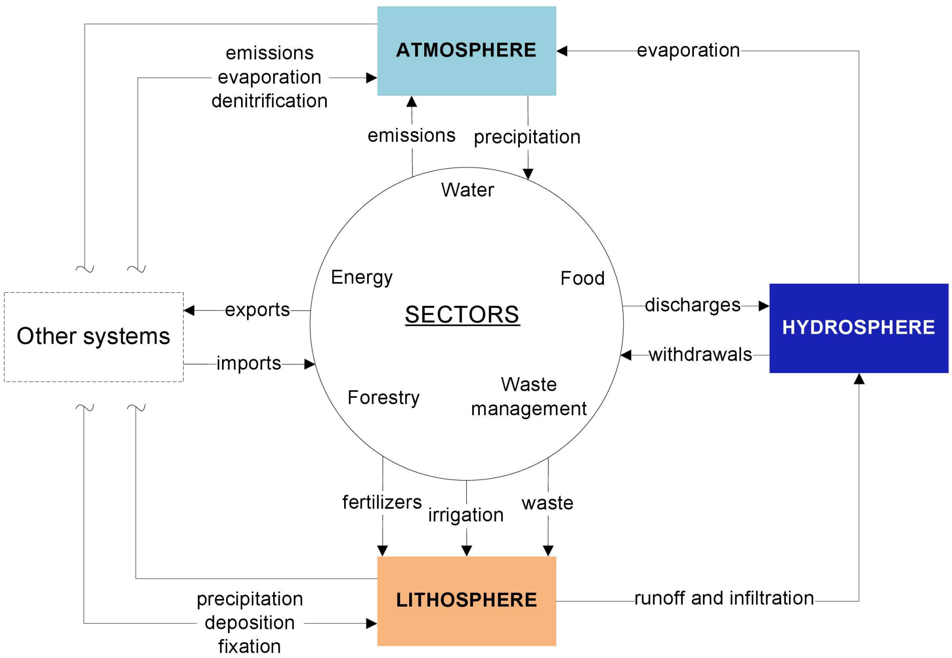

Figure 3.2: Simplified scheme of the multi-sectoral system.

3.1.2 Indicators for the Multi-Sectoral Analysis

The Multi-Sectoral Analysis (MSA) framework includes a set of indicators that allows the assessment of performance in a quantitative way and a means to compare different case scenarios. Imagine the Multi-sectoral system as a black box from the point of view of a substance k with resources R_k entering, and products P_k, wastes W_k, and emissions exiting (aquatic emissions A_k and air emissions E_k). These are aggregated terms calculated as follows (using P_k as an example):

$$\mathrm{P}_k = \sum_{j=1}^{N} \mathrm{F}_k^{j,p} \tag{3.1}$$

where $\mathrm{F}_k^{j,p}$ is the jth flow classified as a product, hence p superscript, of a total of N flows. The substance or species k = 1, 2, 3, 4, and 5 refers to water, nitrogen, phosphorus, carbon, and energy respectively. These substances are often found as part of a material flow so that,

$$\mathrm{F}_k^j = \mathrm{F}^j \cdot \mathrm{C}_k^j \tag{3.2}$$

where F_k^j is the flow of species k as part of the jth flow; C_k^j is the content of substance k in the jth flow, generally as a mass fraction or as units of energy per unit of mass (e.g. $\mathrm{kWh\,t^{-1}}$), in the case of energy. The categorization of flows is performed based on the following definitions:

- *Products* are flows assumed to be resources for processes of other systems, i.e., outside the system's boundaries, and are typically not designated for disposal.
- *Resources* are flows that enter the system as raw materials or finished products for internal use but generated beyond the system's boundaries.

- *Wastes* are basically those flows designated for landfilling as their final disposal method. The specific value is estimated as the material that remains confined within the landfilling chamber after emissions and leaching are calculated. To an extent this flow can be considered an emission to the lithosphere.

- *Air Emissions* are those releases to the atmosphere in either gaseous and aerosol form. It accounts also for fine particles that can be transported by air. In the context of the MSA, this term also includes inputs from the atmosphere, e.g., deposition, so strictly speaking, it refers to a flux.

- *Aquatic Emissions* are flows discharged to either surface or ground water bodies. This mainly refers to non-point source pollution and soil infiltration, or leaching.

The categorization process results in the assignation of the superscripts p, r, w, e, or a, as a reference to products, resources, wastes, emissions to air, and emissions to water respectively. In the more specific context of the Multi-sectoral Analysis (MSA), Table 3.1 offers more detailed information on how specific flows are categorized. Because of phenomenon such as deposition and photosynthesis, the strict definition of E_k is that of a flux that can exit or enter the system.

Following the discussion in Sections 1.3.2 and 2.2, the societal flows classified as described in Table 3.1, can be used for designing a set of indicators to measure the level of eco-efficiency and eco-effectiveness of the system. A total of eight indicators were developed, the first four with focus on eco-efficiency and efficiency concepts, while the remaining four are based on the three tenets of the *cradle-to-cradle* philosophy described in Section 2.2. The first indicator reflects on the overall productivity of the system, i.e., how much product is generated per unit of resource consumed, and can be calculated as in Equation (3.3). This indicator, a measure of efficiency, informs about whether the system is generating more products per unit of resource,

Table 3.1: Flows and possible categorization for the calculation of indicators.

Resources	**Products**	**Air Emissions**	**Water Emissions**	**Wastes**
Fertilizers	Fertilizers	Volatilization	Soil infiltration	Landfilled material
Food	Food	Deposition[a]	Surface runoff	
Fodder	Fodder	Landfill emissions	Landfill leaching	
Compost	Compost	Composting emissions	Composting leaching	
Manure	Manure	MSW[e] incineration		
Wood products[b]	Wood products[b]	Photosynthesis		
Livestock	Livestock	Metabolic respiration[c]		
Biomass (energy)	Biomass (energy)	Firewood combustion		
Fuel[d]	Fuel[d]	Fuel combustion[d]		
Electricity	Electricity	Denitrification		
Potable water	Potable water	Precipitation		
Wastewater	Wastewater	Evapotranspiration		
Water withdrawals	Water discharges			
Inter-basin transfers	Inter-basin transfers			

[a] Includes wet and dry deposition.
[b] Paper, cardboard, and wood.
[c] Calculated for humans and livestock.
[d] Includes coal, gasoline, diesel, biofuels, and natural gas.
[e] Municipal Solid Waste (MSW).

$$\mathrm{PRI}_k = \frac{\mid \mathrm{P}_k \mid}{\mathrm{R}_k} \tag{3.3}$$

where R_k is the sum of resources of substance k entering the system; P_k is the sum of products of substance k being generated and exiting the system; PRI is the productivity indicator. Another measure of the efficiency of the system is the relation between resources used and wastes generated as an indication of the portion of resources entering the system that are converted or lost as wastes.

$$\mathrm{RWI}_k = \frac{\mathrm{R}_k}{\mathrm{W}_k} \tag{3.4}$$

where W_k is the aggregated term of wastes of species k; RWI is the resources usage indicator. Eco-efficiency involves relating the benefits generated by the system (products) and the attaching environmental burden, often represented by the amount of wastes and emissions to the atmosphere and aquatic bodies. Thus, indicators PWI and EEI are elaborated as follows,

$$\mathrm{PWI}_k = \frac{\mid \mathrm{P}_k \mid}{\mathrm{W}_k} \tag{3.5}$$

$$\mathrm{EEI}_k = \frac{\mid \mathrm{P}_k \mid}{(\mathrm{E}_k^{(-)} + \mathrm{A}_k)} \tag{3.6}$$

where $\mathrm{E}_k^{(-)}$ are those emissions to the atmosphere (only in that direction), and A_k represents the emissions released to aquatic bodies. PWI and EEI are eco-efficiency indicators with respect to wastes and emissions respectively. The previous four indicators instrument efficiency concepts, while the following four are designed to implement eco-effectiveness concepts. Indicators HAE and HWE rely on the definition of *healthy emissions* and their comparison with emissions associated with human-managed areas,

$$\mathrm{HAE}_k = \frac{\mathrm{E}_k^0}{\mathrm{E}_k} \tag{3.7}$$

$$\mathrm{HWE}_k = \frac{\mathrm{A}_k^0}{\mathrm{A}_k} \tag{3.8}$$

where E_k^0 and A_k^0 are the healthy emissions of species k between the system and the atmosphere and water respectively, corresponding to the reference state; E_k is the actual net flux of species k between the system and the atmosphere. The perception of good environmental quality changes among regions and over time. For example, from less than 10 parameters, e.g. physical, chemical, and biological, considered in the late 19th century, currently more than 500, including endocrine disruptors and heavy metals, are now being advised for water quality assessment. There are also difficulties for defining a *pristine* water quality state, since some water bodies can be considered *naturally impaired* for a given designated use (Meybeck, 2005). Thus, instead of specifying *healthy emissions*, E_k^0 and A_k^0, based on environmental quality parameters, a desirable flux of nutrients is defined as a reference state that represents the desired sustainable state of the system. This reference state will usually depend on the sustainability objectives proposed for the region. Section 5.2 shows an example of a reference state used for the Upper Chattahoochee Watershed case study.

The indicator WEF embodies the concept of *waste equals food* described by McDonough and Braungart (2002) as a measure of how effective is the system in generating an output flow similar to a calculated *reference* output of materials that the system would generate if all *waste* streams were products, i.e. have a associated benefit,

$$\mathrm{WEF}_k = \frac{\mid \mathrm{P}_k \mid}{\Phi_k} \tag{3.9}$$

where WEF is the *waste equals food* indicator and Φ_k is defined by the following expression:

$$\Phi_k = \mathrm{R}_k - \Delta S_k + \mathrm{E}_k^0 + \mathrm{A}_k^0 \tag{3.10}$$

The term ΔS_k refers to the annual accumulation of species k in all five sectors. Accumulation is calculated based on the flows entering and exiting the system, i.e. resource consumption, production, emissions, and disposal rate of materials, as follows,

$$\Delta S_k = \mathrm{R}_k + \mathrm{P}_k - \mathrm{W}_k + \mathrm{E}_k + \mathrm{A}_k \tag{3.11}$$

Equation (3.11) assumes that accumulation occurs at the rate necessary for fulfilling the demands of the system without judging its adequacy. Finally, a comprehensive eco-effective indicator, described in Equation (3.12), is defined to include the performance of the previous three indicators, including in this way the notions of *healthy air emissions*, *healthy aquatic emissions*, and *waste equals food*:

$$\mathrm{E2I}_k = \beta_{1,k} \cdot (\mathrm{HAE}_k) + \beta_{2,k} \cdot (\mathrm{HWE}_k) + \beta_{3,k} \cdot (\mathrm{WEF}_k) \tag{3.12}$$

The multipliers $\beta_{1,k}$, $\beta_{2,k}$, and $\beta_{3,k}$ are simply a set of aggregation parameters that express the relative level of importance of each term. For instance, if $\beta_{1,k} = \beta_{2,k} = \beta_{3,k} = 1/3$ then all terms have the same importance. A summary of the sustainability indicators is presented in Table 3.2 showing the mathematical objective of the indicator that is associated with a sustainable state.

Table 3.2: Summary of Environmental Sustainability Indicators defined for the Multi-sectoral Systems Analysis framework.

Abbreviation	**Objective**	**Description**
PRI	maximize	Measure of useful products generated within the system per unit of resources consumed
RWI	maximize	Measure of resources consumed per unit of waste for disposal
PWI	maximize	Measure of the amount of products per unit of disposed waste
EEI	maximize	Measure of the amount of products per unit of emission to the environment, either to the atmosphere or water bodies
HAE	unity	Measure of the disparity (ratio) between the actual amount of emissions to the atmosphere and the healthy emission level defined
HWE	unity	Measure of the disparity (ratio) between the actual amount of emissions to water bodies and the healthy emission level defined
WEF	unity	Compares the amount of products versus the quantity that the system would generate if no flows are classified as waste and all emissions correspond to a healthy emission, i.e., waste equals food
E2I	unity	Encloses together the concepts of waste equals food and healthy emissions

As mentioned before, the focus of the MSA is currently on five species k, water, nitrogen, phosphorus, carbon, and energy, and where nutrients are considered regardless of their chemical form or oxidation state. For instance, all the forms of nitrogen released from a process are converted and lumped together as N. Although it is different to release NO_x versus N_2, because of their direct effect on the environment, the MSA approach has a resource perspective. For example, the nitrogen lost to the atmosphere or to a water body was, at some point, part of a resource flow as a result of the use of work and possibly other resources (e.g. the Haber-Bosch process in the case of fertilizers). For this reason, this dissertation includes all forms of N, P, and C.

3.2 The Water Sector

The driving force of the water sector is precipitation. In general terms, once rainfall hits the ground it could either infiltrate, generate rapid surface runoff, or evaporate. A portion of the former produces lateral interflow while the rest recharges the water table. Infiltration is controlled by the infiltration capacity of the land and by the ocurrence of *variable surface areas*. The previous description summarizes the hydrological behavior of a mostly rural area or forest, but human activities can change the hydrology of a region by introducing reservoirs, altering water supply, and constructing impervious surfaces (Kaye *et al.*, 2006). Therefore, when dealing with urban areas, there are other mechanisms that need to be considered. Similar to the model proposed by Mitchell *et al.* (2001) for urban systems, water flows in a partially urbanized watershed can be described by the following representation,

$$W_{precip} + W_i + I_w + I_{ww} = E_t + D + R_o + S_i + \Delta S_w \tag{3.13}$$

where W_{precip} is precipitation; W_i is water withdrawals from surface or ground water sources; I_w and I_{ww} are the net import of finished water and wastewater respectively; E_t is evapotranspiration; D includes discharges to surface water streams or lakes; R_o is surface runoff; S_i is the water infiltrated through soil; ΔS_w is the storage of water within the system's boundaries. Since rivers and lakes are not part of the system, the storage term is typically small. Figure 3.3 is built upon the urban water system described by (Beck, 2005) to include also hydrological processes of urban and rural areas subject to anthropogenic manipulations.

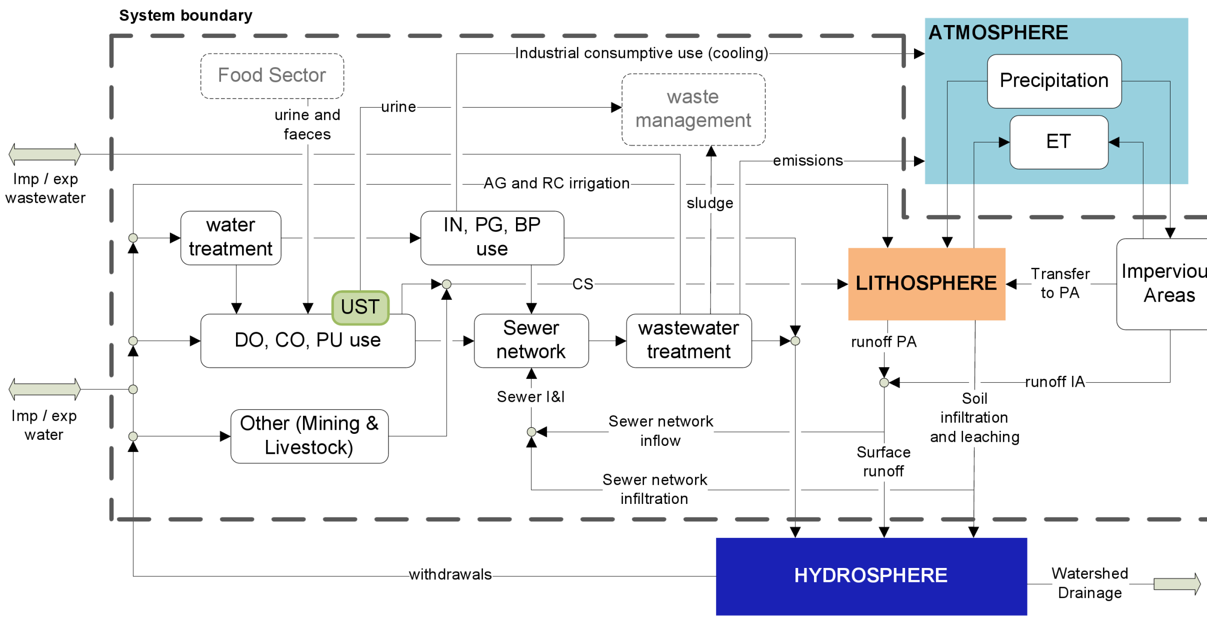

Figure 3.3: Detailed flow diagram of the water sector. Dashed-border boxes denote other systems that receive or deliver flows to the present system. Abbreviations: DO domestic or residential; CO commercial; CS: consumptive use (including septic tanks); PU public; PG power generation; BP biofuel production; IN industrial; ET evapotranspiration; PA pervious areas; IA impervious areas; AG agricultural; RC recreational; UST urine separation technology explained in Section 5.1.

Water withdrawals W_i account for different uses of water: domestic, commercial, public use, industrial, agricultural, and power generation, the last two being the largest water uses, i.e., almost 80% of all fresh water withdrawals. Public water-supply systems, usually maintained by counties or city water departments, make use of surface and underground sources, providing water to 84% of the US population (Hutson *et al.*, 2004). Self supplied water for domestic or residential use is mostly withdrawn from ground-water sources, since it requires minimal treatment. Public supply and self supply are determined by water consumption per capita. Withdrawals for power generation, on the other hand, are a function of the electricity generated, in units such as $m^3\,kWh^{-1}$, and also of the process involved, e.g. coal-fired or natural gas. Water use for livestock operations is calculated based on the inventory (count of heads) of three types of livestock: poultry, cattle, and swine. Withdrawals for the irrigation of agricultural and recreational areas is based on the area irrigated and the corresponding irrigation rate, e.g. in $\mathrm{m\,y^{-1}}$. National data can be used for agricultural areas, see USGS (2009), while for recreational, generally golf courses and parks, available data are usually at the regional level with typical values of the order of 0.7–1.5 $\mathrm{m\,y^{-1}}$ for the southeastern US, see for example SJRWMD (2002, 2004).

E_t includes plant transpiration, evaporation from surface water, evaporation from soil water, industrial evaporation, and evaporation of water stored in impervious surfaces after precipitation events. Long term E_t is controlled by climatological conditions and also by the land cover type. Land cover can be classified into low intensity urban, high intensity urban, crop and pastures, open water and wetland, clear cut and sparse, and forested areas , e.g. (NARSAL, 2006). Accordingly, it is possible to have estimates of the proportion of impervious areas — roads, roofs, and paved surfaces — and pervious areas, grossly categorized into open water, grassland, cropland, and forests. Evaporation from impervious and pervious areas are calculated separately. It is assumed that the water volume retained on impervious surfaces evaporates completely after each precipitation event. The total water stored on an annual basis is calculated therefore as a function of the impervious area retention volume (α_{56}) and the number of precipitation events that take place during the year, reported for example by NCDC (2008). For open water surfaces, and relatively humid pervious areas, the semi-empirical method of Penman is used (e.g. Dunne and Leopold (1978); Doyle (1990). Penman's equation has been used together with a correction factor that accounts for the availability of water due to soil moisture; thus for dry years evapotranspiration will be lower than wet years, for which evaporation approaches its potential rate. Doyle (1990) proposed a fairly simple correction factor as a function of soil moisture deficit with respect a predefined moisture level at which actual evaporation $E_{t,a}$ tends to potential evaporation $E_{t,p}$. In a similar fashion, it is assumed that for long-term estimations, evapotranspiration can be corrected by a moisture factor $M_f = W_{precip}/M_p$ that relates actual annual precipitation W_{precip} and a predefined precipitation level at which $E_{t,a} \rightarrow E_{t,p}$. However, if precipitation is larger than M_p then the correction factor is equal to one ($M_f = 1$).

Discharges from industrial facilities, power generation plants, and municipal wastewater treatment plants are aggregated to calculate D. Similarly to W_i, discharges are a function of consumption patterns and process characteristics. The difference between withdrawals and discharges is regarded as consumptive water use. From the point of view of a watershed, consumptive water is typically defined as the water that is not returned to its source. The pool of water available for infiltration S_i, as defined in Equation (3.13), is the aggregation of the estimated portion of precipitation not lost via runoff — based on an infiltration index — and evaporation plus the first four definitions of consumptive use in the following list:

- Discharges to septic tanks
- Land application of wastewater effluent
- Outdoor watering of gardens and recreational areas
- Agricultural irrigation
- Interbasin transfers
- Evaporation from power generation or industrial use

Water use and consumptive use varies among power generation processes. Under a once-through cooling system — water is pumped from the water body through the heat exchange equipment and then discharged back to the source — a typical thermoelectric coal plant uses about $100\,\mathrm{l\,kWh^{-1}}$, while a natural gas plant can reach $85\,\mathrm{l\,kWh^{-1}}$ of generated electricity. This cooling system usually reports a consumptive use due to evaporation of about $4.0\,\mathrm{l\,kWh^{-1}}$ (Feeley III *et al.*, 2008).

The loss of nutrient via leaching is associated with water infiltration S_i in pervious land. Generally, forest floors are the main source for nutrient leaching (Currie *et al.*, 2003). After nutrients are drained from surficial layers of organic soil, e.g. forest floor, subsequent mineral soil layers act as a physical and biological filter so that most of the nutrient entering the mineral soil is either quickly utilized by soil microorganisms or retained as stabilized mineral-bound organic matter, see for instance Sanderman *et al.* (2008). The mass of the forest floor profile, usually called the O horizon, varies significantly among regions and depends to a great extent on the level of disturbance of the forest. Forests in the South Eastern region of the US can accumulate nearly 62 tonnes of organic matter per hectare, while in Lower Michigan, also about 200 years after the last disturbance, a mass of 12 tonnes per hectare has been reported (Schaetzl, 1994). A similar approach is considered for cropland and grassland, so that by estimating the amount of organic matter in the O horizon, a background leaching concentration of nutrients is estimated before considering the contribution of fertilization supplements.

In low- and high-intensity urban areas, sewer network infiltration and inflow, typically called I/I, is associated with the water infiltrated through soil and surface runoff by an infiltration and inflow index respectively that considers only the urban portion of the system, see Mitchell *et al.* (2001). When water for domestic, commercial, and public use is obtained from surface sources, discharges to septic tanks are considered a consumptive use. Septic tank usage has been related with population density in previous studies. For instance, estimations of the percentage of population discharging to septic systems in the northern region in Georgia, US, was found to follow the expression $87.4 \cdot e^{-0.83 \cdot \rho}$ where ρ is population per acre (JJG, 2003a).

The most process-intensive element of the water sector is definitely the municipal wastewater treatment plant (WWTP). As part of the Multi-Sectoral Systems Analysis, wastewater treatment is calculated as a single process unit for the whole system using an advanced activated sludge treatment scheme. A simplified process flow diagram is presented in Figure 3.4 showing a typical arrangement of equipment. The amount of N losses to the atmosphere due to nitrogen biological removal can be assumed as a proportion of the influent N (Sonesson *et al.*, 2004), and based on a typical plant-wide removal rate, e.g., 85–90% of influent, it is possible to estimate the nitrogen associated with fresh sewage sludge. Since phosphorus has no gaseous phase, plant-wide P removal, typically about 95%, is sufficient for estimating the phosphorus recovered in fresh sewage sludge as well. The flow path of carbon is more complex. For this, it is necessary to model the reduction of Biochemical Oxygen Demand (BOD), cell formation, and cell endogenous decay. In this way, the amount of carbon released as CO_2 in the activated sludge process can be estimated based on the atmospheric oxygen usage, as well as the suspended solids — including volatiles — sent for digestion. The digestion process generates methane gas (CH_4) and carbon dioxide (CO_2) through volatile solids destruction that is recovered for energy uses, mostly heating. Supernatant liquid is separated, carrying a portion of N, P, and C back to the inlet of the plant, while the rest constitutes what is called treated municipal sludge. The flow of treated sludge is directed to the Waste Management sector for further processing or disposal based on the choice specified in the input file. Valuable information with regard to design and operation parameters of WWTPs can be found in Reynolds and Richards (1977).

3.3 The Energy Sector

Energy balances at the urban level have been done mainly from two perspectives: climate (Mitchell *et al.*, 2008) and energy use (Kaye *et al.*, 2006; Hosier, 1993). The former considers natural (primarily solar) and anthropogenic (in the form of heat released) energy fluxes from the climate point of view, to gain insight into how these fluxes affect the water cycle. The second focuses on the use of renewable and non-renewable energy sources and what are the drivers for such consumption. The MSA couples both approaches, since these two can reveal information about how efficiently the rural-urban system uses available energy sources and

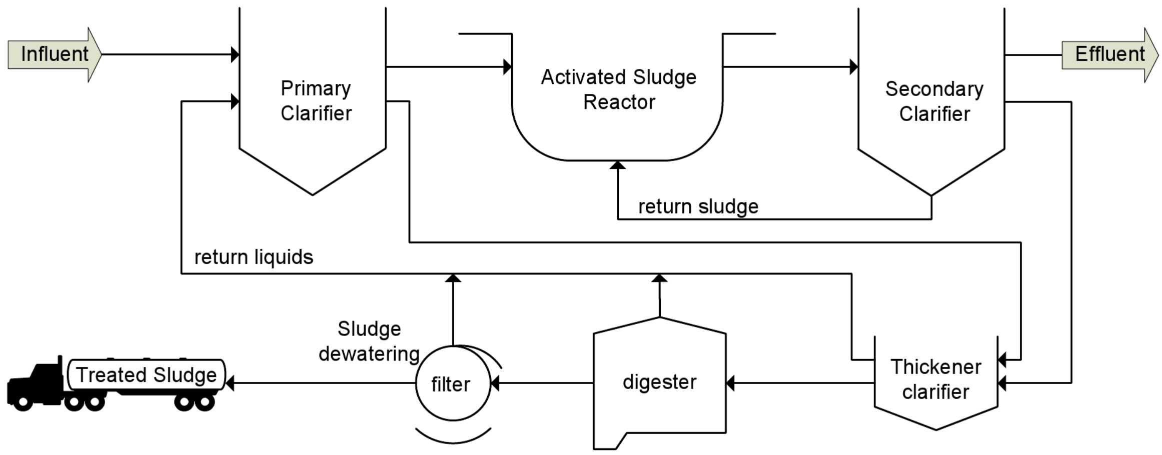

Figure 3.4: Simplified process flow diagram of a WWTP based on an activated sludge process scheme.

how much of the energy that arrives from the sun finds a productive use. Equation (3.14) describes the urban model for heat flows without consideration of anthropogenic heat fluxes (Mitchell *et al.*, 2008; Grimmond and Oke, 2002).

$$Q^* = Q_E + Q_H + \Delta Q_S \tag{3.14}$$

where Q^* is the net all-wave radiation; Q_H is the turbulent sensible heat flux from the ground surface; Q_E is the latent heat flux lost due to evaporation and transpiration; and ΔQ_S is the net heat storage by land and other surfaces such as pavement and buildings. However, this storage occurs only during daytime, and most of the heat is lost via convection and radiation during the night. Thus, the terms Q_H and ΔQ_S are understood as a resource flow available mostly during the daytime. The terms in Equation (3.14) are estimated using information on land-surface characteristics and weather observations. Q_H and Q_E have been expressed in a parametrized form as a function of $(Q^* - \Delta Q_S)$ (Grimmond and Oke, 2002), which after manipulation results in,

$$\frac{Q_H + \beta}{Q_E - \beta} = \frac{1}{\alpha} \cdot \left(1 + \frac{\gamma}{s}\right) - 1 \tag{3.15}$$

where α and β are empirical parameters. The former depends on terrain characteristics as shown in Table 3.3, while the latter is typically $20\,\mathrm{W\,m^{-2}}$ for rural regions and $3\,\mathrm{W\,m^{-2}}$ for urban areas. The term γ/s is the inverse of the Penman's parameter where γ is the psychometric constant $0.66\,\mathrm{mb\,°C^{-1}}$ and s is the slope of the saturation vapor pressure versus temperature (Dunne and Leopold, 1978).

Table 3.3: Values of the empirical parameter α for different landscapes (Grimmond and Oke, 2002).

Landscape	α
Dry desert (no rain)	0.0–0.2
Arid rural area	0.2–0.4
Crops and field (dry)	0.4–0.6
Urban, some parks	0.5–1.0
Crops, fields, and forests (sufficient soil moisture)	0.8–1.2
Lakes and oceans (land more than 10 km distant)	1.2–1.4

The net all-wave radiation can be calculated based on how much radiation arrives at the land surface, how much is reflected, and how much is lost as long wave radiation.

$$Q^* = Q_{SR} \cdot (1 - albedo) - Q_{LW} \tag{3.16}$$

where Q_{LW} is the net long wave radiation and Q_{SR} is the solar radiation received on a horizontal plane corrected by the value of reflectivity, also known as *albedo*. Reflectivity is a specific property of a material, in this case, of the surface terrain (Prado and Ferreira, 2005). Q_E can be calculated from the actual amount of water vaporized,

$$Q_E = M_E \cdot \lambda_w \tag{3.17}$$

where M_E is the mass of water evaporated in kg and λ_w is the water heat of vaporization, i.e., $1.0\,\mathrm{kcal\,kg^{-1}}$. The energy balance presented so far refers only to the rural-urban energy cycle from the climate perspective, and energy fluxes are directly associated with solar input, radiation, and the latent heat in water evaporation from land and pervious surfaces. The energy balance that accounts for power generation and fuels is described in Figure 3.5.

As of 2005, the world's energy demand was about 139 PWh, of which 86% was satisfied by fossil fuels, 6% from nuclear fuels, and the remaining 8% includes biomass, hydropower, solar, wind, and other alternative energy sources. End users, demanding fuels or electricity, to a total of 920 GWh for the State of Georgia as an example, can be classified into various activities: domestic, commercial, industrial, and transportation. The proportion among these activities in the State of Georgia, USA, is 23, 18, 29, and 30% respectively; however, this varies depending on the economic and technological characteristics of the region. In the US, 60% of households rely mostly on electricity, while 40% uses a combination of electricity and natural gas, in a ratio near 50:50. A less significant fuel demand at the residential level corresponds to firewood, with a US average of firewood consumption is $0.2\,\mathrm{m}^3$ per capita (Howard, 2007). The commercial sector uses electricity, natural gas, and with a larger magnitude compared to the domestic sector, biomass. The industrial sector adds coal to its sources, besides electricity, natural gas, and biomass. Transportation, on the other hand, is

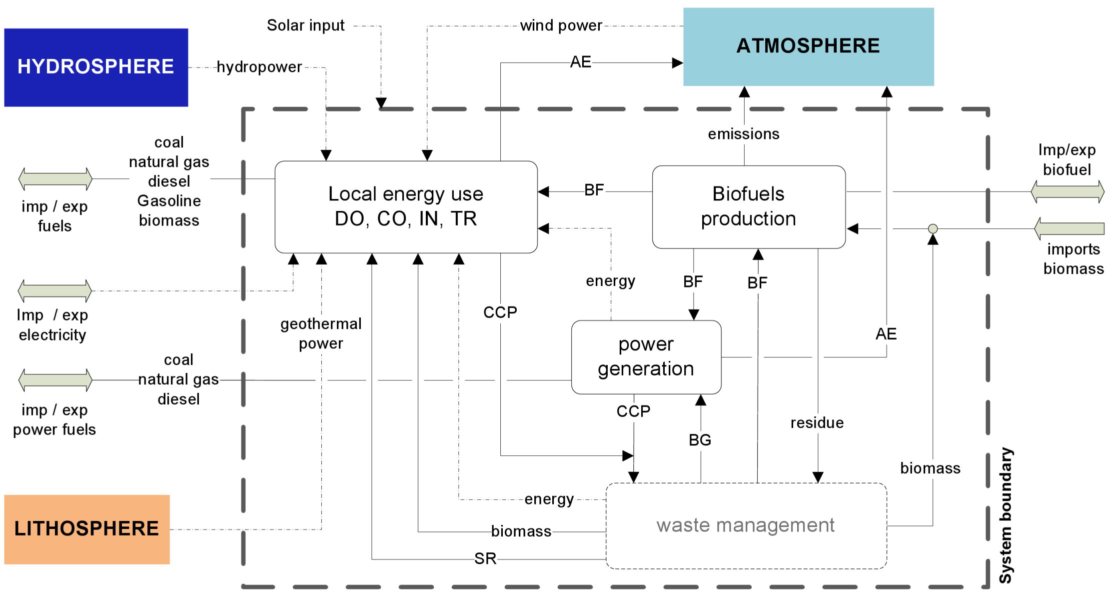

Figure 3.5: Detailed flow diagram of the energy sector.The dashed-dotted line (– · · – ·) represents an energy flow with no mass value. Dashed-border boxes denote other systems that receive or deliver flows to the present system. Abbreviations: DO domestic or residential; CO commercial; IN industrial; TR transportation; BF liquid biofuel; BG biogas; AE air emissions; SR sawmill residue.

mainly based on gasoline, diesel, and natural gas. Summarizing, the direct sources of energy for electricity, heating, and transportation considered in the MSA are listed in Table 3.4.

Table 3.4: Energy sources and fuels considered by the Multi-sectoral Systems Analysis categorized into renewable and non-renewable.

Renewable	**Non-renewable**
Liquid biofuels (e.g. biodiesel)	Coal
Gaseous biofuels (e.g. biogas)	Natural gas
Biomass and firewood	Diesel
Wind power	Gasoline
Hydro-power	Nuclear
Geothermal	Import electricity[a]
Import electricity[a]	

[a] Rather than a fuel or an actual energy source, when imported, electricity is viewed as an energy carrier that can come from renewable or non-renewable origins.

Indirectly, the Waste Management sector can generate heat or electricity from processes such as the incineration of municipal solid waste (MSW), explained in Section 3.5.2, and landfill gas capturing, described in Section 3.5.4. The model accounts for the flow of fuels as materials based on the requirements of the system, usually expressed as the amount of energy (kWh) required to accomplish an activity. The next step is to establish the energy source for each type of activity. Converting an energy source into available work is associated with a level of efficiency, and in the case of electricity, a distribution loss factor, which in the US is about 2.16. By accounting for these two elements, it is possible to estimate the real need of fuels. For example, a power plant will need to generate 316 GWh to effectively deliver, at the user site, 100 GWh, and if the generation is coal-powered, assuming that coal has an energy value of $9000\,\mathrm{kWh\,t^{-1}}$ and a process efficiency of 0.35, the required mass of coal required is about 100 tonnes. A part of the energy sector model deals with the estimation of emissions from the different types of fuels. The estimation for liquid and gaseous fuels is more or less straightforward and 100% oxidation is assumed (IPCC, 2006b). A more complex approach is required for biomass and coal. Biomass, assumed to have typical wood properties, has an ash content of between 0.75 and 2.5% (FAO, 1986), and a portion of the biomass nutrient content remains in the ash, particularly minerals such as P.

Potential CO_2 emissions from coal combustion power plants are typically in the order of 320 kg of CO_2per MWh (Hong and Slatick, 1994). Roy *et al.* (2009) estimated an emission factor based on mass of coal, resulting in about 1.45 kg CO_2 per kg of coal. The Intergovernmental Panel for Climate Change (IPCC) reports a value of $25.8\,\mathrm{t\,C\,TJ^{-1}}$. In all cases, CO_2 emissions correspond to values close to full oxidation of carbon content in coal. Hower *et al.* (2005) report, based on an ultimate analysis of coal combustion residue, less than 3% of carbon in bottom ash and boiler slag. These two by-products, plus fly ash and flue gas desulfurization (FDG) material, are usually called *Coal Combustion Products* (CCP), which are produced at a rate of nearly 33 kg per 100 kg of coal burnt (Butalia *et al.*, 1999). Because most of the world's power generation depends on coal combustion, i.e., some 50% of it (EIA, 2010), CPPs cannot be ignored; thus there has been extensive studies to give valuable uses to CCPs (Ahn and Mitsch, 2002; Sajwan *et al.*, 2006). About 0.5–1% of the particles released to the atmosphere (Mahowald *et al.*, 2008), at a rate close to 4–110 mg per kWh of generation (Ohlström *et al.*, 2000), is phosphorus, while the rest remains as CPP. The mechanisms by which coal combustion releases nitrogen species are more complex. NO_x emissions from coal combustion depend on the nitrogen content of coal, usually between 0.6 and 2.3% dry ash-free (Kambara *et al.*, 1995), but only 75% to 90% is associated with the fuel-bound nitrogen, while the rest is provided by oxidation of combustion air (Baxter *et al.*, 1996). A better way to estimate how much fuel-bound N has evolved as gas is to correlate this to coal's mass loss during combustion. Baxter *et al.* (1996) corroborated in their experiments that N mass loss in coal combustion is proportional to the overall coal mass loss (in a dry ash-free basis) but smaller by a factor 1.25–1.50. The assumed final mass after coal combustion is equal to the mass of CPP recovered.

3.4 The Forestry and Food Sectors

These two sectors have similar behavior in the sense that most of their activity takes place in the soil environment before being sent to consumers. Figures 3.6 and 3.7 show the processes that are being considered and the flows interconnecting them. Soil nutrient processes are addressed in conjunction with the forestry and food sectors based on the description of nutrient cycles in Section 2.3. In forest and crop land, inputs of C are reflected in the increase of C stocks in above-ground and below-ground biomass, see Equation (3.18). At the level of the forestry sector, the import of wood products, such as paper, cardboard, lumber, and firewood, are added to the inputs. Outputs can be characterized by the CO_2 release from dead organic matter (DOM), soil organic matter (SOM), and harvested wood products that are exported to other systems. Logging residue can be sent to the Waste Management sector for further processing or left on-site, in which case plant C becomes part of the soil carbon pool with the potential for accumulation or release as CO_2. Carbon cycling associated with biomass is estimated based on the recommendations set out by IPCC (2006a), which accounts for different types of land use, including forests, grassland, and cropland. Thus,

$$\Delta C = \mathrm{A} \cdot G_w \cdot (1 + R_{ab}) \cdot C_{fract} \tag{3.18}$$

where ΔC is the change in carbon stock; A is the area of interest; G_w is the average annual above-ground biomass growth; R_{ab} is the ratio of below-ground to above-ground biomass; C_{fract} is the mass fraction of carbon, typically 0.4–0.5. Within the forestry sector there are three main units considered: forest production, internal wood processing (depicted as *sawmills*), and local consumption. The internal use of wood products can be grouped into timber products, firewood, and pulpwood products. In 2000, the average consumption per capita in the US was 2.0, 0.2, and 0.67 m^3, respectively (Howard, 2007). The consumption that is not covered by internal production, dependent on very specific industrial characteristics of the region, is supplemented by imports. Waste wood products are sent to the Waste Management system for recovery or disposal. About 44–50% of the municipal solid waste (MSW) generated is associated with wood products and biomass such as paper, yard trimmings, and construction materials (RWBECK, 2005; EPA, 2009). The flows of water, nitrogen, phosphorus, and energy are estimated using Equation (3.2). Wood-based materials have a low moisture content, so that the contribution to the water cycle from these products is expected to be minimal. Moisture in air-dried timber varies usually between 12 and 20% (USDA, 1973), but paper, newspaper, and cardboard will not exceed 0.5% in mass.

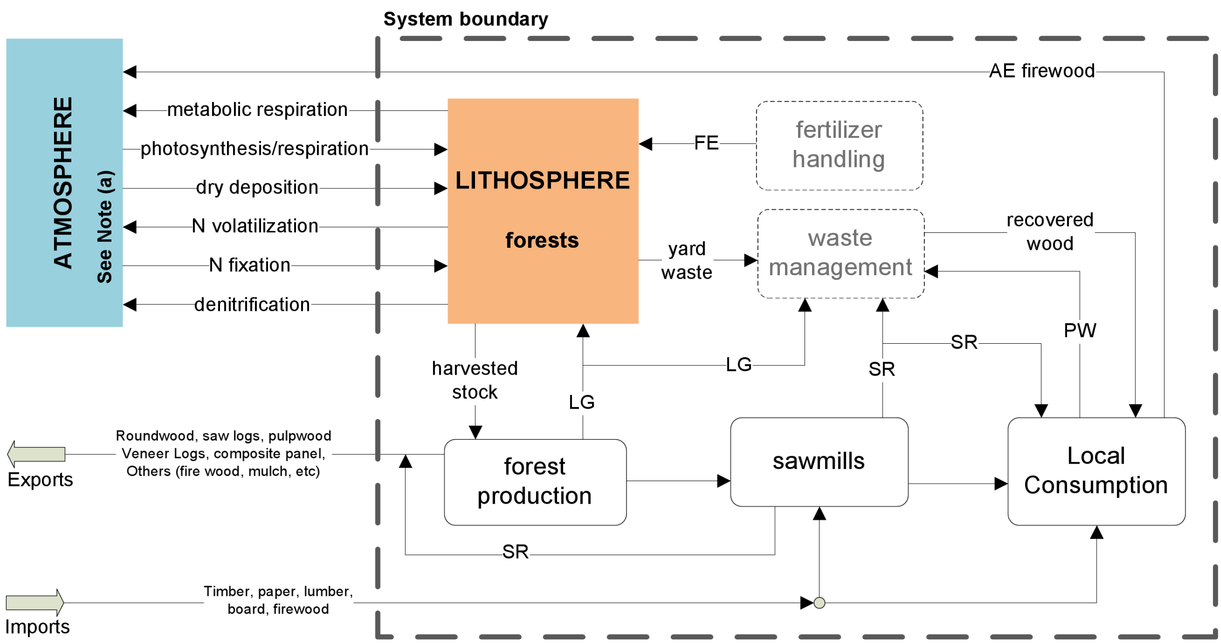

Figure 3.6: Detailed flow diagram of the forestry sector. Dashed-border boxes denote other systems that receive or deliver flows to the present system. Abbreviations: LG logging residue; FE fertilizers; AE air emissions; SR sawmill residue.
Note (a): Flows between the lithosphere and the atmosphere, such as plant respiration and photosysthesis, N volatilization, denitrification, deposition, and N fixation include those flows corresponding to the food sector (see 3.7).

The estimation of required fertilizers for the three types of representative land uses, i.e. grass, crop, forest, based on regional or national data (Reicher and Throssell, 1998; Landry *et al.*, 2002; USDA, 2008), is used to establish an internal consumption value and, from that point, the imports of fertilizer are calculated, see Equation (3.19). The same procedure is employed to determine the amount of resource or product that is imported or exported, respectively.

$$M_{ie} = M_{consumed} - M_{produced} \tag{3.19}$$

where M_{ie} is the material imported (positive value) or exported (negative value); $M_{consumed}$ is the amount of material consumed; $M_{produced}$ is the material produced within the system (locally). In general, the flows calculated by the model follow this rule: a negative value is an outgoing flow while a positive value refers to an incoming flow. For example, the production rate of manure for each type of livestock is well documented, see Table 3.5, thus it is possible to estimate the mass of manure generated within the system if the inventory of livestock is known.

Table 3.5: Annual manure production rate of livestock based on body mass (James *et al.*, 2006).

	kg manure/body weight kg
Poultry	16–32
Cattle	30–32
Swine	10–30

There are several practices for providing additional nutrients to soil, identified by the type of nutrient source used, (i) inorganic fertilizers, chemically synthesized, and (ii) organic fertilizers, such as treated sewage sludge, poultry litter, and manure from cattle and swine. When organic matter is utilized as a source of nutrients for crops or forests, particularly in the case of N and P, the availability of these nutrients needs to be considered for the calculation of the amount of manure to be applied. Typically *Plant Available Nitrogen* (PAN) requires a complex calculation that accounts for the mineralization rate of organic nitrogen and the degree of retention of inorganic nitrogen, in the form of nitrate-N (NO_3-N) and ammonium (NH_4-N). PAN has shown a strong dependency on the carbon-to-nitrogen ratio (C/N), i.e., a higher C/N will result in lower PAN values. Manure handling and/or treatment have a significant influence on the C/N ratio, hence on PAN as well. Fresh material typically shows higher PAN values than composted material (Gale *et al.*, 2006). For instance, fresh poultry litter can reach a PAN of 60%, with an average of about 30%, but after composting, nitrogen will not be available at a rate higher than 10% and averaging 5% (Gale *et al.*, 2006; Preusch *et al.*, 2002; Tyson and Cabrera, 1993). Nitrogen availability of plant material, e.g., yard trimmings and crop residuals, is much lower than that found in manure, usually on the order of 10–15% before, and about 2% after, composting. Food refuse behaves similarly to manure and sewage sludge (Sullivan *et al.*, 2002). Although composting reduces the availability of nutrients to plants, it is a necessary process for some organic materials to reduce nutrient and pollutant losses via runoff or leaching, minimize nuisance odors, reduce vector attraction, destroy pathogens, and also prevent immobilization of inorganic nitrogen in soil (Sullivan *et al.*, 2004; Cogger *et al.*, 2002). For municipal sludge, a value of 40% availability has been used (Lundin *et al.*, 2004).

In the case of *Plant Available Phosphorus* (PAP), values are typically higher than PAN with respect to the total content of the nutrient in manure. Laboratory analysis of composted manure has shown that P is lost via runoff and leachate, particularly in open composting facilities (Eghball *et al.*, 1997), but due to the high proportion of inorganic phosphorus in animal manure, a large part of the P is readily available for plant utilization. PAP has been found to be about 70% for poultry litter (Eghball *et al.*, 2005) and sludge applications (Lundin *et al.*, 2004). As opposed to inorganic sources, which in principle allow better proportioning of nutrients by the mixing of different fertilizers, organic fertilizers have a nutrient ratio, e.g. N:P, that does not necessarily correspond to the estimated crop uptake; therefore, some of the nutrients supplied to the soil are often in excess and more prone to be transported via hydrological processes.

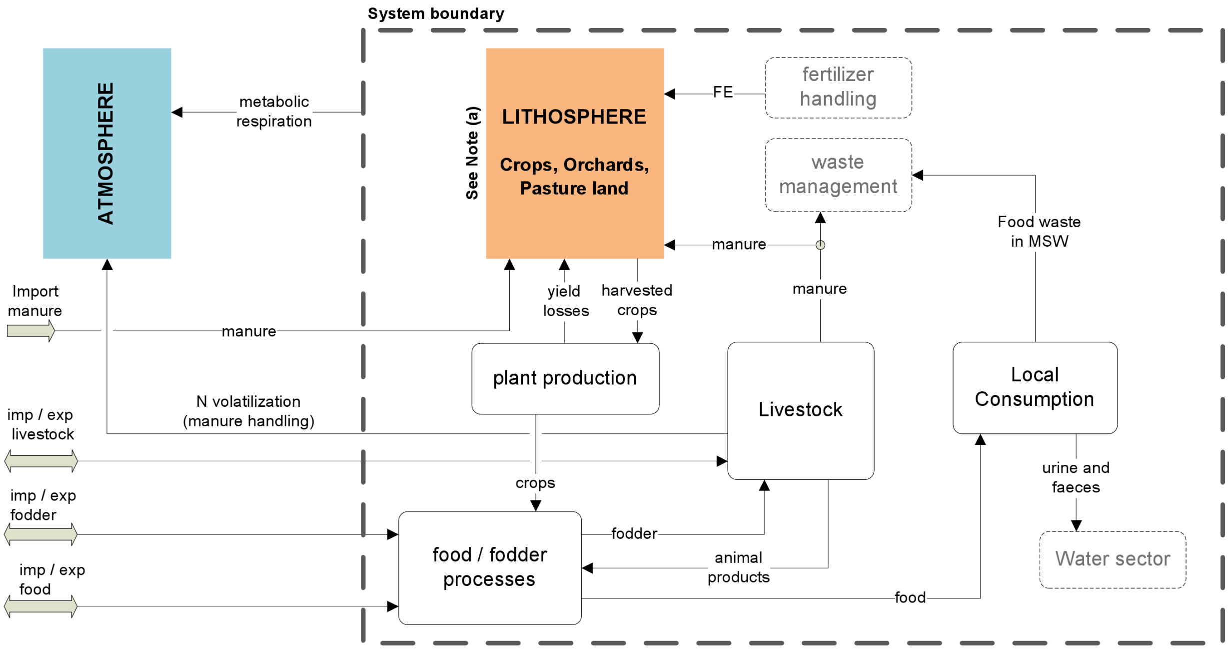

Figure 3.7: Detailed flow diagram of the food sector. Dashed-border boxes denote other systems that receive or deliver flows to the present system. Abbreviations: FE fertilizers; MSW municipal solid waste.
Note (a): Flows between the lithosphere and the atmosphere, such as plant respiration and photosysthesis, N volatilization, denitrification, deposition, and N fixation are all aggregated as part of the forestry sector in Figure 3.6.

Despite the many similarities between the forestry and the food sector, the latter has a larger variety of input flows, accounting in this way for imports and exports of food, fodder, livestock, and manure, which are calculated after internal production is estimated using Equation (3.19). Food has been classified into representative groups as a way to organize the food categories reported by the Food and Agriculture Organization of the United Nations (FAO). Table 3.6 shows consumption patterns in the US for the year 2000 (FAO, 2009a) for each representative group of food. These values are comparable to those reported by Sahely *et al.* (2003). Food waste, typically 10–14% of MSW, is sent to the Waste Management sector.

Table 3.6: Food consumption per capita in the US for the year 2000.

Food group	**Consumption ($\mathbf{kg\,y^{-1}}$)**
Fruits	125
Cereals	116
Vegetables	207
Meat (bovine, swine, poultry)	121
Fish/Seafood (seafood, freshwater fish)	23
Dairy (milk, butter, ghee, eggs)	272
Others (alcoholic beverages, vegetable oil, stimulants, sugar and sweeteners)	206

Feed consumption by livestock is based on animal inventory and digestible energy (DE) requirements, usually estimated in $\mathrm{kcal\,d^{-1}}$ per head, as recommended by NRC (1987). Based on the feed, DE will determine the amount of dry mass to be fed (e.g. corn, hay). Nutrient supplements will be required to comply with specific requirements for minerals (phosphorus in this case) and additional protein, the largest nitrogen contributor in food (NRC, 1961, 1998, 2000).

Metabolic respiration of livestock, and humans too, is often ignored. However, Prairie and Duarte (2007) report an estimated global $0.6\,\mathrm{Gt\,C\,y^{-1}}$ associated with human respiration, and $1.5\,\mathrm{Gt\,C\,y^{-1}}$ with livestock. If these values are compared to the current total emissions from fossil fuels ($9\,\mathrm{Gt\,C\,y^{-1}}$), it becomes quite significant, and even more if indirect emissions due to excretory decomposition ($1.0\,\mathrm{Gt\,C\,y^{-1}}$) are added. Decomposition of feces and manure is considered in processes related to wastewater treatment and losses from manure handling, storage, and composting; thus the model includes explicitly only metabolic respiration by an allometric relation based on Prairie and Duarte (2007),

$$M_R = 3.32 \cdot {B_w}^{0.79} \tag{3.20}$$

where M_R is the metabolic respiration in $\mathrm{kg\,C\,y^{-1}}$ and B_w is the body mass in kg.

3.5 The Waste Management Sector

The waste generated in all the previous sectors is handled in the Waste Management sector (WMS) as the ultimate barrier between human activities and the environment, see Figure 3.8. This sector is the most complex of all due to the various process-intensive units present in it, with a total of six: sludge digestion, solid waste incineration, composting, MSW landfilling, struvite production, and solid waste pyrolysis. The first four are described in the present section, but the last two (highlighted in green in Figure 3.8) are treated as a modification to the structure of the system, i.e., a *structural change*, compared to what is considered the business-as-usual scheme. These two waste management units are explained in Section 5.1. The underlying purpose of the structure of the WMS is: recovering energy and recovering material with a fertilizer value. In both cases, the objective is to produce flows that can be classified as *products*. The inputs to this sector are municipal solid wastes, wastes generated from the wastewater treatment process, manure from livestock operations, yard waste, and CCP from coal-powered plants. MSW is the largest component, with a generation rate of 1.2–2.5 $\mathrm{kg\,d^{-1}}$ per capita (Arena *et al.*, 2003; RWBECK, 2005), but this varies enormously among regions. The variability is evident in the composition of MSW as well.

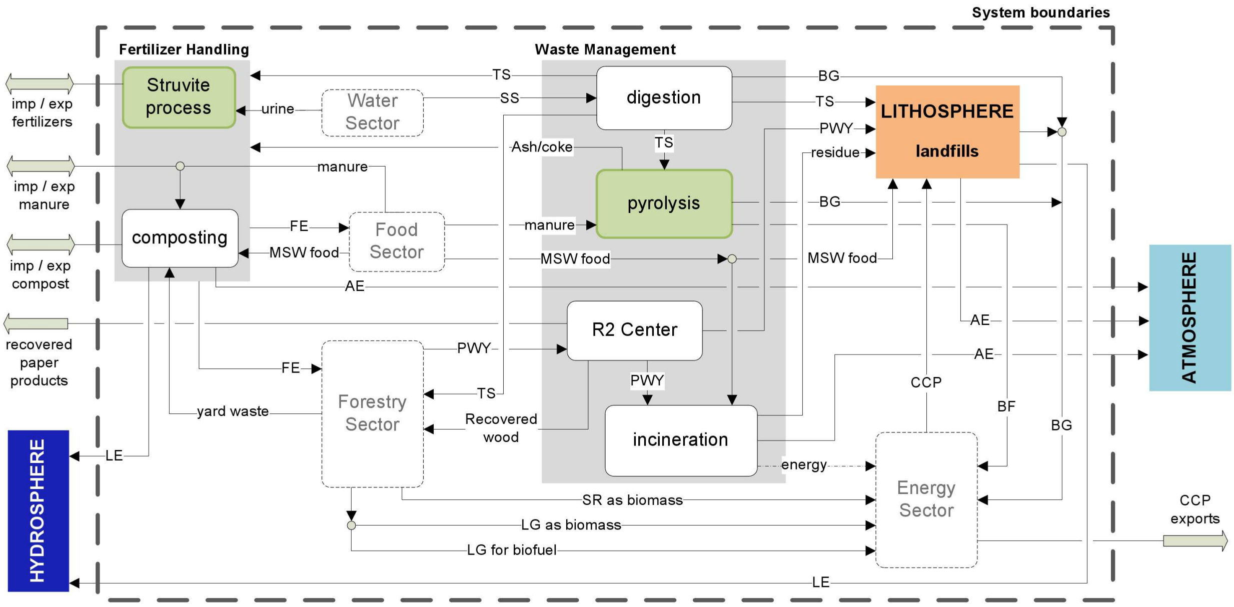

Figure 3.8: Detailed flow diagram of the waste management sector. Dashed-border boxes denote other systems that receive or deliver flows to the present system. Green-highlighted boxes represent technologies that are put in place as a structural change, as explained in Section 5.1. Abbreviations: BF liquid biofuel; BG biogas; AE air emissions; MSW municipal solid waste; R2 recycling and reusing; TS treated municipal sludge; SS fresh municipal sludge; SR sawmill residue; FE fertilizers; LG logging residue; LE leaching; CCP coal combustion products.

3.5.1 Municipal Sludge Digestion

The main purpose of the digestion process is to reduce the solid mass weight and reduce pathogen activity by oxidation of degradable organic material. The process is carried out by microbes under very specific process conditions of temperature and oxygen availability. Most of the digestion processes perform nearly at atmospheric pressure, so it is typically not a factor to account for. The digestion process considered in this work is a thermophilic reactor under anaerobic conditions, which can be summarized by the following chemical expression,

$$\mathrm{OM} + \mathrm{Oxygen} \xrightarrow{Anaerobic\ microbes} Cells + E + \mathrm{CH_4} + \mathrm{CO_2} + Others \tag{3.21}$$

where OM is organic matter and E is energy for cells. Oxygen is mainly provided by radicals such as carbonates (CO_3^{-2}), nitrates (NO_3^{-1}), sulphates (SO_3^{-1}) and phosphates (PO_4^{-3}); *Others* refers to traces of N_2, H_2S, and water vapor. Sludge cells can be represented as a chemical formula to facilitate calculations of gases produced during digestion. Such a chemical formula can be derived from the ultimate analysis of treated sludge resulting in Table 3.7 (Thipkhunthod *et al.*, 2005; Khan and Daugherty, 1992). The availability of data in the form of an ultimate analysis makes possible the calculation of the energy value of organic matter, which is also applicable to manure flows.

Typically 50–75% of the volatile organic matter in sludge, which corresponds to 65–75% of the total amount of solids, is destroyed by the digestion process, resulting in the production of CH_4 and CO_2 in a proportion that varies with the performance of the microbes, but normally in the 1.2–3.0 range of CH_4:CO_2. The gas production rate ranges from 1.05 to 1.75 kg per kg of volatile solids degraded (Reynolds and Richards, 1977), with a heating value calculated as a function of the volume of CH_4 characterized by having $10.34\,\mathrm{kWh\,m^{-3}}$ at

Table 3.7: Typical characteristics of treated sludge on a dry basis.

	Atomic Subscript[a] (average and range)	**Content**[b] (weight %)
C	5 (4.12–6.61)	28.6–34.0
N	0.4 (0.25–0.75)	1.5–3.3
H	8.5 (6.6–10.6)	-
S	0.09 (0.01–0.20)	-
O	1.8 (0.38–3.03)	-
P	-	0.12–4.1

[a] Source (Thipkhunthod *et al.*, 2005; Channiwala and Parikh, 2002)
[b] Source (Houillon and Jolliet, 2005; Gascó and Lobo, 2007)

standard conditions. This gas can be recovered and used as fuel for heating the digestion process itself and other units within the WWTP complex.

3.5.2 Municipal Solid Waste Incineration

A typical MSW incineration unit will release 0.7–1.2 tonnes of carbon dioxide per tonne of waste. This figure makes no distinction between biogenic and fossil carbon, the latter being 33–50% of the total C released (Johnke, 2000). The portion of MSW considered by the model includes food, wood products, and yard residue, thus the emission of gases is calculated with similar considerations to those of the biomass combustion, explained in Section 3.3. The energy produced depends on the energy content of the materials incinerated and the process efficiency.

3.5.3 Composting

Manure, discarded food, and yard waste are the typical feed for composting. The result is a stable material, i.e. no nuisance odors, no vector attraction, and no pathogens, with still some nutrient value. The efficiency of the composting process depends on the C to N ratio (ideally 10–30) and humidity (50% desirable). The species in the composting process are partitioned through leaching, air emissions, and solid state (the mass that remains in the composted material. Water losses via evaporation are typically 30–80% (Balkema, 2003), so that there are occasions when the composting operation requires water addition. A total mass loss is usually 35–50% but the presence of soil within the compost material reduces the apparent mass loss (Eghball *et al.*, 1997). Reported values of losses of each nutrient, via leaching, are below 2% of the initial mass. Table 3.8 summarizes the experiences drawn from previous studies, serving as a basis for partition factors for N, P, and C. However, the losses of P, presumably via leaching, seems excessive, even when compared with land application of composted municipal sludge, which are less than 1% (Esteller *et al.*, 2009).

3.5.4 Landfilling

As for the composting process, landfilling involves the decomposition of material and releases of nutrients to the water table and atmosphere. The model assumes that 100% of the produced leaching is loss through the soil and that a portion of the gas — set in the input file — is captured for energy purposes. Table 3.10 shows reported values of nutrient compositions of MSW and concentrations in leachate. Compared with the composting process, the landfilling model uses a more flexible approach for estimating leaching of nutrient. Raveh and Avnimelech (1979) elaborated, under simulated conditions, a set of empirical equations for the estimation of C and N concentration in leachate over time with an exponential form,

$$N_c = a \cdot b^t. \tag{3.22}$$

Table 3.8: Composting losses of mass and nutrients via leaching and air emissions together.

	Losses as mass percentage[a]		
	Cattle manure[b]	**Corn stalks and hog manure**[c]	**wood- or straw-bedded and Cattle manure**[d]
C	45–62	42–68	34–53
N	22–42	37–60	11–42
P	0.8-2.2	23-39	-
Total mass	15–20	34–55	26–30
Initial C:N	12–18	9–12	17–36
Final C:N	8–11	14–21	13–26

[a] In all cases composting was performed in windrows.
[b] Source (Eghball *et al.*, 1997).
[c] Source (Tiquia *et al.*, 2002).
[d] Source (Hao *et al.*, 2004).

where N_c is the nutrient concentration in leachate in $\mathrm{mg\,l^{-1}}$; a and b are empirical parameters; t is time in years. Using the Composition of MSW, it was possible to correlate the nutrient input to the landfill with the mass of nutrient lost in leaching. By adapting data generated by Scott *et al.* (2005), a similar equation is possible for phosphorus. The resulting parameters are presented in Table 3.9.

Table 3.9: Empirical parameters for landfill leaching for nitrogen, phosphorus, and carbon[a].

	a	**b**
N	0.29	0.54
P	0.29	0.59
C	0.09	0.51

[a] The use of the parameters follows Equation (3.22) which results in a partition coefficient in kg of nutrient leached per kg of nutrient landfilled, e.g. kg C/kg C in refuse.

Table 3.10: Composition and leaching of landfilled MSW for nitrogen, phosphorus and carbon.

	Composition[a] **(weight %)**	**Leaching concentration**[b] **($\mathrm{mg\,l^{-1}}$)**
C	33-47	30–29000
N	1.0–3.0	70–5700
P	0.055–0.110	0.1–23

[a] Source (Raveh and Avnimelech, 1979; Sørum, 2000).
[b] Source (Ehrig, 1983; Kjeldsen *et al.*, 2002).

The calculation of gaseous emissions from a landfill is based on the LandGEM model developed by Alexander *et al.* (2005) for the USEPA. This method calculates the amount of CH_4 based on: (i) the mass of waste (tonnes), (ii) a methane generation rate ($\mathrm{y^{-1}}$), (ii) and a value of potential methane generation ($\mathrm{m^3\,t^{-1}}$). Once the amount of CH_4 has been estimated, it is possible to estimate the total amount of carbon (CH_4+CO_2) and nitrogen by using a typical composition of landfill gas (see Table 3.11).

Table 3.11: Landfill gas composition (% volume) from US and other countries after Scott *et al.* (2005).

	US	**Other**
CH_4	44.0–53.4	45–60
CO_2	34.2–47.0	40–60
N_2	3.7–20.8	2.0–5.0

3.6 Applying RSA to the MSA

The details of the RSA procedure itself were presented in Section 2.4, while its interaction with the MSA is graphically described in Appendix C. In the context of this research work, RSA is incorporated into the MSA framework so that the information generated is useful even if the information provided to the model contains a degree of uncertainty; however, there are three specific purposes in mind,

- Accounting for uncertainty propagation from model parameters and inputs to the output of the model.
- Establishing whether targets — expressed as a degree of improvement of an environmental sustainability indicator — are possible, given the structure of the model.
- Identifying those parameters — and consequently those flows, processes and sectors associated with them — that are *key* or *critical* for reaching proposed targets.

Uncertainty of data, expressed as an interval, is sometimes available, but the lack of information is more often the case. In an SFA study of heavy-metals in Stockholm, Hedbrant and Sörme (2001) proposed a set of uncertainty levels based on the quality and the applicability of different sources of information. This approach was also applied later to study the nitrogen flows in a Swedish municipality (Danius and Burström, 2001). Table 3.12 summarizes these uncertainty levels that are implemented in the MSA framework. RSA makes use of the intervals calculated with the uncertainty levels to sample the parameter space and generate possible model output values. Instead of using the traditional uncertainty interval expression $\{\pm u_j\}$, it is proposed to express uncertainty as a factor such as $\{*/u_j\}$ which results in an asymmetrical interval. For example, if a factor of $u_j = 2$ is used, then the parameter space is defined by $[\frac{1}{2}\overline{\alpha}_j, 2\overline{\alpha}_j]$, where $\overline{\alpha}_j$ is the most likely value of parameter α_j.

Table 3.12: Uncertainty level classification based on the source the parameter information based on Hedbrant and Sörme (2001).

Level	**Interval factor(*/)**	**Source of information**
1	1.10	Official statistics and literature values at the local level
2	1.33	Official statistics and literature values (local) at the regional and national levels.
3	1.50	Simulated data for the area of interest (local)
4	2.00	Official statistics and literature values at the regional and national levels downscaled to the local level.
5	4.00	Global and general information

Because of its procedure, in which the Kolmogorov-Smirnov test is performed on each parameter individually assuming that they are statistically independent, RSA is considered a univariate method. Therefore, there are two types of parameter correlation that must be discussed. The first is correlation on the input side, that is, when the value of two or more parameters are correlated because of the nature of the process these parameters are describing. For instance, in a food web model 'food intake' can be linked to 'growth rate' in the sense that a low value of 'food intake' can be related to a low 'growth rate'. For this reason the modeling platform of the MSA tries to consider parameters that are independent of each other. The second type of correlation, particularly in very complex models, can take place on the output results side, that is, the sensitivity of the model output (the indicators) to a parameter can be diminished or enhanced by the behavior of another parameter. The possibility of parameters appearing irrelevant for the model (diminishing effect) has been acknowledged in other studies (Grieb *et al.*, 1999; Bastidas *et al.*, 1999; Osidele, 2001; Arabi *et al.*, 2007). However, a larger parameter vector-size (a large number of sampling iterations) enhances the statistical robustness of the RSA results (Bastidas *et al.*, 1999). On the other hand, satisfying the condition $f_m(\alpha_j|B) \neq f_n(\alpha_j|NB)$ is sufficient to conclude that the model is sensitive to the parameter α_j. However, this should be considered as a first step towards understanding the level of criticality of a parameter. Additional information can be generated about the hierarchical importance of the $\{B\}$ parameters with respect to the behavioral space by implementing the Tree-Structured Density Estimation (TSDE) method, e.g. (Osidele, 2001).

The present chapter explains each one of the industrial sectors involved in the MSA structure, but the assessment of how this structure performs under different conditions is up to the indicators formulated in Section 3.1.2. Because the MSA makes use of large amounts of data, management of uncertainty becomes prominent, and for this, the RSA procedure is employed. These three elements are put into practice in a triplet of case studies, starting in Chapter 4, by performing a flow and energy accounting exercise, applied to the Upper Chattahoochee Watershed, as a way to enhance the understanding of the capabilities of the MSA framework.

Chapter 4

CASE STUDY PART I: System Metabolism

"It is the mark of an instructed mind to rest satisfied with the degree of precision which the nature of the subject admits and not to seek exactness when only an approximation of the truth is possible." Aristotle

Following the description of the five sectors comprising the MSA in Chapter 3, it is time to explore its capability for estimating material and energy fluxes entering, exiting, and within a partially urbanized watershed. As an accounting exercise, this offers understanding of which are the more relevant fluxes in terms of magnitude, and possibly, which sectors are the most dominant in the region. This case study Part I, used for illustrating the usefulness of the MSA framework, includes mass — nutrients — and energy accounting as a way to gain insight into the characteristics of the metabolism of the Upper Chattahoochee Watershed. This chapter presents what herein is called the *base case* as a way to have a sense on the magnitude of flows of the system and upon which the study case Part II (sustainability performance) and Part III (reachability of targets) are built.

4.1 The Upper Chattahoochee Watershed

The capabilities of MSA are exemplified in the context of the Upper Chattahoochee Watershed (UCW) located in north-central Georgia, in the south-eastern USA, see Figure 4.1. Nearly a quarter of the Metropolitan Atlanta area is within this watershed. By 2000, the population of the Upper Chattahoochee Watershed was about 1.3 million. The major surface water storage in Georgia, Lake Sidney Lanier, is located just north of Atlanta within the limits of the UCW. The lake is also the principal source of drinking water for the metropolitan Atlanta area. Table 4.1 shows the concentration of nutrients in the lake. The watershed area, a total of 4093 km^2, is comprised of the Appalachian Mountains to the north, and low to high intensity urban areas to the south. It has a variety of land uses including significant poultry production and silviculture. In 2000, land cover was categorized as follows: open water 4%, forest 53%, urban and sub-urban 29%, pasture and crops 10%, other 4%. As an extension of the discussion initiated in Section 2.1.6, it is presumed that considering a large area, one that includes both urban and agricultural activities, for instance, offers better opportunities for improving nutrient and energy cycles.

There are arguments in favor of and against considering a system at the watershed level. On the one hand, detailed data are mostly available at the state or county level, which does not necessarily match the boundaries of a watershed; thus, it is necessary sometimes to adjust data using factors derived from population, household number, land use, or surface area. However, on the other hand, the water cycle is much more manageable when considering a watershed and nutrient cycling has been an extensively studied topic for watersheds. Although in principle the MSA methodology is applicable to any system, the UCW is of strategic importance for the region, not only because of the economic-intensive activity that takes place within it, but also because the health of the Chattahoochee River, originating in the UCW and flowing through the Metro Atlanta area, has vital relevance to three states (Georgia, Alabama, and Florida).

About 88% of the Upper Chattahoochee Watershed is located in the Piedmont area and only 12% in the Blue Ridge. With a moist and temperate climate, the UCW receives an annual average of 1270 mm of precipitation, primarily during the winter and early spring. The average monthly temperature in the Metropolitan Atlanta area ranges from about 7 to 26°C (Chapman and Peck, 1997).

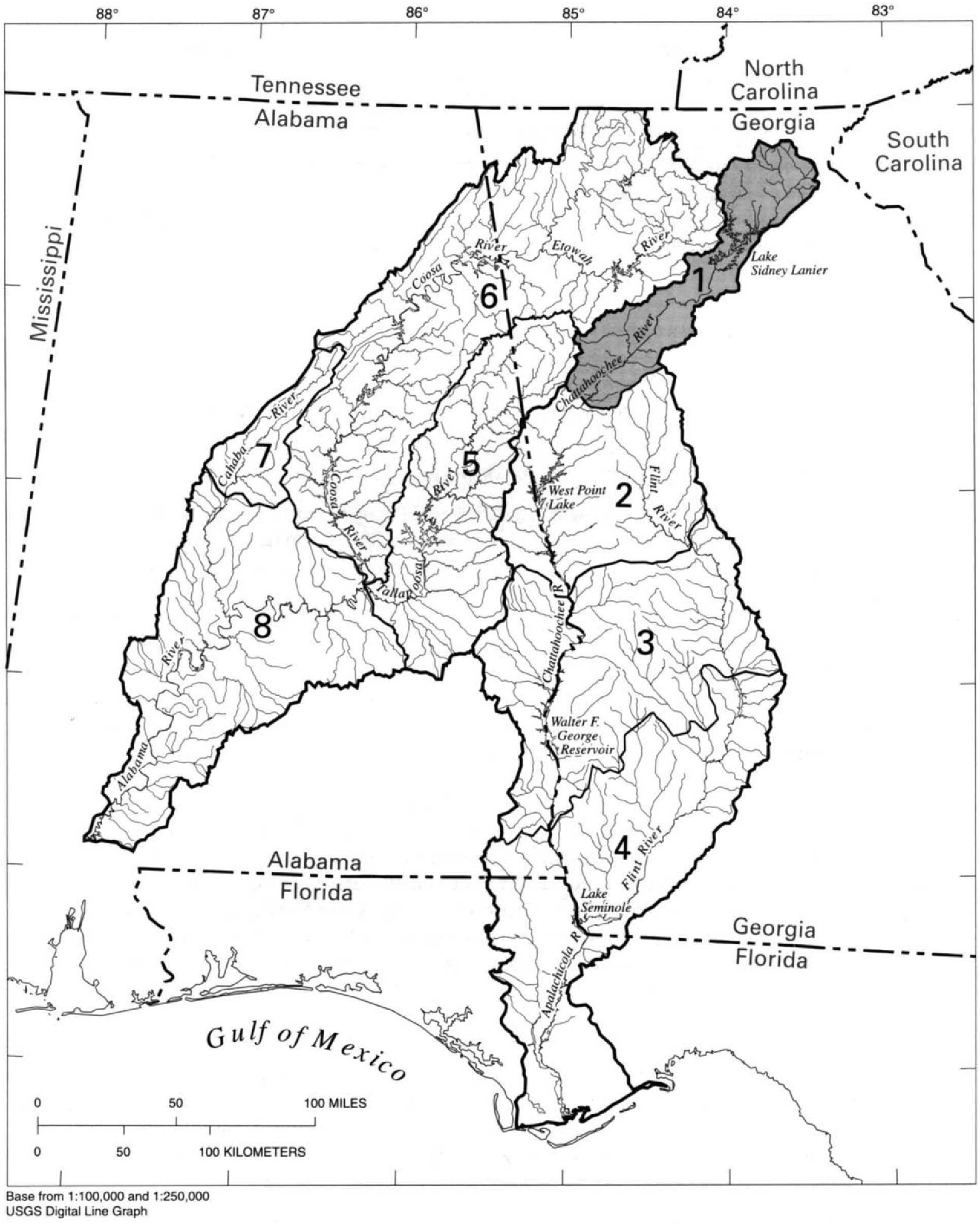

Figure 4.1: Subareas and major streams in the Apalachicola-Chattahoochee-Flint and Alabama-Coosa-Tallapoosa River Basins in the USA (Chapman and Peck, 1997). The Upper Chattahoochee Watershed is highlighted and numbered as *Subarea 1*.

Table 4.1: Nutrient concentrations in Lake Lanier, the major source for drinking water for the Metro Atlanta area (Zeng and Rasmussen, 2005).[a]

	Concentration (mg l^{-1})		
	Mean	**10th percentile**	**90th percentile**
TKN	0.270	0.130	0.500
TP	0.012	0.004	0.032
TOC+TIC	6.850	3.270	10.27

[a] See Appendix A for chemical symbols and abbreviations.

4.1.1 Data Sources

The magnitude of material flows can change significantly from one region to another due to differences in consumption patterns, process efficiencies, land use, and other factors. Therefore, efforts were made to use data specific to the Upper Chattahoochee Watershed, when available. Most of the data are retrieved from official sources such as the Environmental Protection Agency (EPA), Georgia Department of Natural Resources (GA DNR), US Department of Agriculture (USDA), US Geological Service (USGS), the US Census Bureau, the Food and Agriculture Organization of the United Nations (FAO), and the Intergovernmental Panel on Climate Change (IPCC). Specific water-quality data, collected by the USGS, are available at the USGS National Water Information System (NWIS). Energy information is found at the state and national level at the official website of the Energy Information Agency (EIA). The rest of the information is retrieved from literature found in agency reports, journals, and extension agencies publications.

4.1.2 Region-specific Aspects

It is important to know some of the hydrological characteristics of the UCW, such as typical river discharge and baseflow, so that the range assumed for the parameters α_{64} 'watershed relief' — used for calculating baseflow contribution (Santhi *et al.*, 2008) — and α_{59} 'pervious area infiltration index' — used for estimating surface runoff — are within the correct order of magnitude. The closest USGS monitoring station to the discharge point of the watershed is station #02336000, located in the Chattahoochee River at Atlanta, GA. At this station, the mean, annual stream discharge is $67\,\mathrm{m^3\,s^{-1}}$, with a range between 41 and $125\,\mathrm{m^3\,s^{-1}}$. Baseflow, on the other hand, ranges from 34 to $90\,\mathrm{m^3\,s^{-1}}$. The unit-area mean, annual baseflow has been simulated as $0.016\,\mathrm{m^3\,s^{-1}\,km^{-2}}$. Mean annual baseflow in the Chattahoochee River is about 69–82% of mean annual stream discharge (Chapman and Peck, 1997).

In forested areas, the surficial layers of the floor, i.e. Oi, Oe, and Oa layers with a total depth of about 10 cm, contain 532 and $9.1\,\mathrm{g\,kg^{-1}}$ of C and N respectively, as reported for a 24-yr-old loblolly pine plantation located at the Whitehall Forest of the University of Georgia, near Athens, GA (Kissel *et al.*, 2009). The O horizon mass in the same forest was found to have a density of $61\,200\,\mathrm{kg\,ha^{-1}}$. These values are similar to those presented by Cortina *et al.* (1995) for a mature *Pinus Radiata* stand located near Barcelona, Spain, exhibiting a lower forest density of about $40\,000\,\mathrm{kg\,ha^{-1}}$, however. The phosphorus content in these three layers had an average of $585\,\mathrm{mg\,kg^{-1}}$, but other studies have shown almost twice that value, $1070\,\mathrm{mg\,kg^{-1}}$, for Isle Royale National Park in Michigan (Rutkowski and Stottlemyer, 1993).

Although more than 50% of the UCW area is forested, human interventions in the watershed's water cycle are not insignificant, with over 500 National Pollutant Discharge Elimination System (NPDES) facilities. Consumptive use of water is an important component of water withdrawal. For instance, about $5.7\,\mathrm{m^3\,s^{-1}}$ (130 million US gallons per day) were reported as the net inter-basin transfer of finished water from the portion of the Chattahoochee

Watershed located within the Metropolitan North Georgia Water Planning District (JJG, 2003b). Similarly, over 1.7 $m^3\,s^{-1}$ (40 million US gallons per day) of wastewater from other basins where treated in the Chattahoochee Watershed. The wastewater unit process was simulated with a known concentration of sewage entering the R.M.Clayton plant, the major wastewater treatment facility in the watershed, assumed to contain domestic, commercial, public, and industrial discharges (see Table 4.2). In the same region, approximately 17% of wastewater generated is handled by septic systems, varying significantly from county to county as a function of population. In more populated counties such as Fulton County and Dekalb County, about 10% of households use septic tanks, whereas in northern areas, e.g., Habersham County, septic systems can be found in 40–90% of the households (JJG, 2003b).

Table 4.2: Typical concentration of nutrients in the influent of the R.M. Clayton Wastewater treatment plant (Mines Jr *et al.*, 2004).

	Concentration (mg l^{-1})		
	average	**minimum**	**maximum**
N	25	16	40
P	4.0	2.50	9.0
BOD	170	110	220

Electricity generation within the UCW is based on three processes: thermoelectric coal plant, thermoelectric natural gas plant, and hydrolectric. The McDonough Power Plant, operated by Georgia Power, has been migrating from its originally coal-only based generation to natural gas. Hydroelectric power is being generated from two dams, Morgan Falls with a nominal capacity of 11 MW, which results in circa 95 $GWh\,y^{-1}$, and Buford Dam with a about 100 MW of generation capacity, which enables the delivery of nearly 870 $GWh\,y^{-1}$. Morgan Falls, built in 1904, regulates the Bull Sluice Reservoir which has a full pond surface area of 2.7 km^2 and is licensed to Georgia Power. Buford Dam, finished in 1956, contains Lake Sidney Lanier with its surface area of 150 km^2 at full capacity and is operated by the US

Army Corps of Engineers. The nominal generation capacity of each process is listed in table 4.3. The 2007 EIA report for GA shows the individual monthly consumption of domestic, commercial, and industrial users of electricity. Based on this, and considering the State's population, it is possible to estimate a value of consumption per capita, which results in 5.9, 4.9, and 3.6 $\mathrm{MWh\,y^{-1}}$ for domestic, commercial, and industrial purposes, respectively.

Table 4.3: Summary of power generation facilities within the Upper Chattahoochee Watershed.

Location	**Process**	**Capacity**[a] **MW**	**Operated by**
Cobb County	Coal-fired	500	Georgia Power
Cobb County	Natural Gas	80	Georgia Power
Fulton County	Hydroelectric	11	Georgia Power
Forsyth County	Hydroelectric	100	USACE[b]

[a] Nominal capacity.
[b] US Army Corps of Engineers.

An important driver of the watershed economy is the livestock industry, represented to a large extent by the production of poultry. By the year 2000, based on data released by USDA (2004), the estimated inventory of poultry birds was 23 million heads, while for cattle and swine this was 60 and 20 thousand heads respectively. With more than 50% of forest, silviculture activity is also relevant. Estimations derived from reports by Thompson (1998) indicate that the annual growth of softwood and hardwood within the watershed is about 3.7 and 4.5 $\mathrm{m^3\,ha^{-1}\,y^{-1}}$ respectively. Removal rate is estimated as 5.8 $\mathrm{m^3\,ha^{-1}\,y^{-1}}$ for softwood and 2.9 for hardwood.

4.2 Results and Discussion

The following sections present the results obtained from applying the MSA framework to the Upper Chattahoochee Watershed with data for the year 2000. Although the analysis includes discussion about the similarities and differences of the behavior among the five species, the results are organized by species. Most of the material discussed is presented in a tabular format, but it is typical in substance flow analysis (SFA) to find results in a more graphical presentation, such as in flow diagrams. As an example, Appendix D shows the material flows of nitrogen corresponding to the *base case* as they pass through the five industrial sectors.

4.2.1 Water

The most dominant flows are associated with climate and natural processes. Precipitation enters the system at a rate of $147.2\,\mathrm{m^3\,s^{-1}}$, of which $94.7\,\mathrm{m^3\,s^{-1}}$ or 64%, is returned to the atmosphere by evapotranspiration. Calculated soil infiltration is $35.5\,\mathrm{m^3\,s^{-1}}$, about 24% of the amount received as rainfall. About $15.3\,\mathrm{m^3\,s^{-1}}$ is estimated as surface runoff, from pervious and impervious areas, that reaches the stream channel. Total water withdrawals are $42.2\,\mathrm{m^3\,s^{-1}}$, including for power generation ($18.3\,\mathrm{m^3\,s^{-1}}$), and inter-basin fresh water transfer ($14.2\,\mathrm{m^3\,s^{-1}}$). Inter-basin transfer may seem high, but it reflects the loss of storage volume from Lake Lanier, a loss of over 2 m of water level, accentuated by the drought that took place in 2000. Water withdrawals for supply of drinking water for domestic, commercial, public, and industrial use are $8.8\,\mathrm{m^3\,s^{-1}}$, of which about 56% is for residential purposes, which is consistent with other populated areas (Grimmond and Oke, 1986). The contribution of water flows in manure and food are not relevant at the watershed level, with calculated values $< 0.5\,\mathrm{m^3\,s^{-1}}$.

Table 4.4 lists the twenty most relevant flows in the water sector and their estimated standard deviation as generated by the Monte Carlo sampling of the parameter space. Most of the SFA studies do not report the uncertainty associated with the estimated flows, presented here in the form of variability; however, this information is critical when used for decision-making purposes. Public water supply is $240\,\mathrm{t\,y^{-1}}$ per capita, which is similar to the water metabolism parameter reported by Kennedy *et al.* (2007) for a typical average city in the

US, 230 t y^{-1} per capita. However, wastewater returns are much higher (277 t y^{-1}) compared to 180 t y^{-1}. The reason for this is the amount of inflow and infiltration estimated by the model. The data from Kennedy *et al.* (2007) are from 1965, when infiltration was probably less significant as a result of newer sewer network; thus, a recalculated wastewater return with no infiltration results in a much closer value, 179 t y^{-1}.

4.2.2 Nitrogen

Agriculture and fuel consumption are responsible for the largest nitrogen flows. Feed for livestock is the major component, at 27 800 t N y^{-1}, of which only 3% is produced in the UCW. Poultry production accounts for 83% of the total use of feed. Consequently, manure production is quite significant at 16 100 t N y^{-1}, 75% of which is from poultry. Storage and handling of manure facilitates the volatilization of about 5400 t N y^{-1}. Some 3500 t N y^{-1} of manure are used for fertilization and the rest (7200 t N y^{-1}) is exported to adjacent areas. Most of the fertilization relies on inorganic sources, all imported, estimated at 3500 t N y^{-1}. Only poultry litter is considered for land application for a total of 3500 t N y^{-1} as well. Remember that the nutrient value of organic sources is based on PAN and PAP (see Section 3.4), but the amount reported is based on the total content of nutrient.

Almost 90% of the food production in the system is based on meat production, 9300 t N y^{-1}, a value comparable, in N terms, to the total food consumed 9500 t N y^{-1}. Consumption of food is 47% meat (bovine, pig, poultry) and 27% cereal products, the rest is vegetables and seafood, 18%, and to a less extent, fruits and dairy, 4%. The intake of food results in the production of urine (5000 t N y^{-1}), feces (1400 t N y^{-1}), and about 1100 t N y^{-1} as food refuse. The first two are collected in the sewer network and processed by the WWTP, where nitrogen is released to the atmosphere (5500 t N y^{-1}) by denitrification. WWTP effluent is responsible for transporting about 1500 t N y^{-1}, while the produced and treated municipal

Table 4.4: List of the twenty most relevant water flows ranked by volumetric flow; the UCW in the year 2000.

Flow description[a]	**Mean value**[b] **($m^3\,s^{-1}$)**	**Standard deviation ($m^3\,s^{-1}$)**
Total precipitation	+147.2	8.6
Total water evaporation	(94.7)	9.8
Total water withdrawals	+42.1	2.2
Total soil infiltration	(36.6)	6.7
Total water returned to surface sources	(29.9)	2.2
Other water returns to surface sources (IN and PG)	18.5	2.1
Water withdrawals for power generation	18.3	2.0
Water withdrawals for power generation - Coal	16.4	2.0
IBT of fresh water	(14.2)	0.5
Surface runoff that reaches the river	(13.3)	1.8
Wastewater returns from WWTPs (effluent)	11.4	0.9
Water withdrawals for public supply	8.8	0.5
DO water use	4.9	0.5
Wastewater from DO, CO, PU to WWTPs	6.3	0.5
Inflow / Infiltration to sewer system	4.1	0.7
CO water use	2.1	0.1
Total consumptive use to soil	1.9	0.1
IN water use	1.4	0.1
Wastewater from industrial uses to WWTPs	1.0	0.1
DO Septic tanks return	0.6	0.0

[a] IN industrial; PG power generation; DO domestic,; CO commercial; IBT inter-basin transfer; WWTP wastewater treatment plant. For a complete list of abbreviations see Appendix A.

[b] Values in parenthesis are flows exiting the system, values preceded by the '+' symbol are entering the system, and the rest are internal flows of the system.

sludge accounts for 3000 t N y^{-1}. Part of the N in urine and feces, about 1000 t N y^{-1}, is lost as part of what in Table 4.5 is called 'soil infiltration' due to the use of septic tanks.

As mentioned before, the use of fuels is second in overall relevance for N flows, but first in emissions to the atmosphere. Local consumption — excluding power generation — is about 27 000 t N y^{-1}. Of these emissions, 55% are released by industrial operations, 29% from commercial, 13% by residential, and 3% from transportation. Because transportation relies mostly on gasoline, which has a low content of nitrogen compared to natural gas, it has a low effect on N flows. Industrial fuel, on the other hand, is based on natural gas, coal, and biomass, hence its large contribution to N emissions. The large standard deviation associated with local fuel consumption is due to the level of uncertainty assigned to the consumption per capita for each user. In the case of power generation, of the total of coal imported into the system, 26 500 t N y^{-1}, nearly 90%, is used for power generation purposes. The combustion process releases 76% of the N in coal, 17 900 t N y^{-1}, while the rest, 6300 t N y^{-1}, is retained within coal combustion products (CCP); 65% of CCP is estimated to be landfilled.

Hydrological processes have a moderate significance for the system's N metabolism. Surface runoff transports a total of 3600 t N y^{-1} to the Upper Chattahoochee river, largely from impervious areas (70%). The total riverine export is about 10 400 t N y^{-1}, or 25 kg N y^{-1} per hectare, which is within the range reported by David and Gentry (2000) of 5–25 kg N ha^{-1}y^{-1} for Illinois, US. Similar values were also obtained by Boyer *et al.* (2002) for a similar region, i.e. 10% urban and 50% forested, even though the input of N in fuels was not considered. Schilling and Zhang (2004) estimated an average of 26 kg N y^{-1} per hectare, only nitrates, for an agricultural watershed in Iowa where 2/3 of the stream concentration was baseflow contribution. Soil infiltration of N, which accounts for leaching from agricultural land, leaching from landfills, and septic tanks results in 4100 t N y^{-1}. Atmospheric deposition of N can represent nearly 4250 t N y^{-1}, of which 77% is wet deposition.

Table 4.5: List of the twenty most relevant nitrogen flows ranked by mass flow; the UCW in the year 2000.

Flow description[a]	**Mean value**[b] **($t\,N\,y^{-1}$)**	**Standard deviation ($t\,N\,y^{-1}$)**
Feed consumption by livestock	27813	1899
Emissions from Local Fuel Consumption	(27060)	7777
Imports of Coal	+26488	2655
Imports of NG	+25958	8458
Total Emissions from Power Generation	(20239)	2013
Fresh manure generated	16106	2599
Total nutrient applied to soil for fertilization	13070	755
Food consumed	9488	334
Food produced	9361	925
Inorganic fertilizer applied	9097	601
Nitrogen biological denitrification	(6835)	1328
Relevant Material Landfilled	6800	684
Coal Combustion Products	6377	639
Air emissions from Wastewater Treatment Plants	(5554)	1529
Nitrogen losses from manure handling (volatilization)	(5397)	905
Total Urine generated	5021	935
Total nutrient deposition	+4252	688
Total soil infiltration	(4134)	340
Surface runoff that reaches the river	(3616)	909
Nitrogen biological fixation	+2713	652

[a] NG natural gas; PG power generation; WWTP wastewater treatment plant. For a complete list of abbreviations see Appendix A.
[b] Values in parenthesis are flows exiting the system, values preceded by the '+' symbol are entering the system, and the rest are internal flows of the system.

Surprisingly, despite the regional importance of the forestry industry, wood-associated flows are within the largest in the system. Tree harvesting produces effectively about 600 $t\,N\,y^{-1}$, after logging residue, while the total consumption of wood products including lumber, paper, and firewood is about 2000 $t\,N\,y^{-1}$. Landfilled waste of wood-pulp products, e.g. paper and cardboard, amounts to 810 $t\,N\,y^{-1}$, while about 680 $t\,N\,y^{-1}$ is recycled. Landfilled material — including municipal sludge, food, wood products, Municipal Solid Waste (MSW) combustion residual, and CCP — adds up to a total of 6800 $t\,N\,y^{-1}$.

Finding that the food and the energy sectors are involved in the largest flows of N in the system is consistent with the work done by Antikainen (2007). However, it is difficult to compare exact flow magnitudes as systems can be radically different, e.g., differences in power generation practices, agricultural activities, or waste management strategies. Yet, for comparison purposes, it is possible to generate intensive characteristics of the system (analogously to intensive properties such as density or concentration) that can be reported independently from the size or magnitude of the system, e.g. sewage produced per capita. Table 4.6 compares data generated by MSA with the results by Antikainen (2007).

4.2.3 Phosphorus

The largest flows of phosphorus are related to feed for livestock and fertilizer use, and to a lesser extent to fuel flows and hydrological processes (see Table 4.7). About 6300 $t\,P\,y^{-1}$ enter the system as feed, with 90% being dedicated to the poultry industry. Consequently, manure is the second most important flow with 4100 $t\,P\,y^{-1}$, and again, 90% is produced by poultry operations. Poultry litter represents 44% of the total nutrient supplied to soil, 3600 $t\,P\,y^{-1}$, while 36% is covered by inorganic fertilizer. Some 95% of the phosphorus in locally produced food is contained in meat products; therefore, the similarity of the terms *food produced* and *food consumed* does not mean that the region is self-sufficient, nutritionally speaking. Meat exports amount to 900 $t\,P\,y^{-1}$, so that local meat production covers a significant portion of

Table 4.6: Comparison of intensive system characteristics of nitrogen. All values reported on a per capita basis.

	MSA ($\mathbf{kg\,N\,y^{-1}}$)	**Other Studies** ($\mathbf{kg\,N\,y^{-1}}$)
N in household wastewater	2.7–7.2	5.2[a], 5.9[b]
Municipal organic waste	0.7–1.1	1.0[a]
Food consumption per capita	6.8–7.8	6.5[a], 6.4[b]
Refuse food (as a percentage of consumed food)	8–15%	14%[a]
Use of fodder	18–24	23[a]
NO_x and elementary N from fuels	23–57	30[a]
N in WWTP effluent	0.4–1.9	1.5[b]

[a] Source (Antikainen, 2007).
[b] Source (Forkes, 2007), scenario for year 2001.

local consumption, which is 50% of the population diet. Cereal and dairy consumption are 21 and 13% respectively.

Approximately 240 $t\,P\,y^{-1}$ of the food consumed is returned as waste, and most is sent for landfilling, but accounting only for 8% of the total material landfilled. Coal combustion products (CCP) are more significant, contributing 39% of the total phosphorus landfilled. Paper and wood products provide 14 and 12% of P each, but 46% of the paper waste generated is recovered before reaching the landfill. Wood recovery, on the other hand, is negligible. Almost all the phosphorus that enters the system in coal, 90% for power generation purposes, is recovered as CCP, but only 35% finds an alternative use, avoiding in this way being landfilled. Some of the treated municipal sludge generated in WWTPs is sent as a soil conditioner or nutrient supplement, but most of it, 63%, is part of the 3200 $t\,P\,y^{-1}$ sent to landfills.

The Upper Chattahoochee river exports about 1800 t P y^{-1} in different chemical forms, equivalent to 4 kg P y^{-1} per hectare, and 70% of this is contributed by non-point sources from agricultural land and urban areas. The export of phosphorus per hectare is relatively high compared to studies by David and Gentry (2000), 0.3–1.0 kg P y^{-1}, Baker and Richards (2002), about 0.3–1.4 kg P y^{-1}, and Pedrozo and Bonetto (1987), 3.1 kg P y^{-1}. Large values in runoff P from the model derive from the assigned value, and its associated range of uncertainty, of the 'phosphorus runoff factor', α_{211}, and the 'surface runoff concentration from impervious areas', α_{232}. The results of Baker and Richards (2002) also indicate that 83–90% of the phosphotus export is generated from non-point sources. Only 6% of the total exported is discharged by WWTPs, comparable to Antikainen (2007), while the rest is mostly associated with baseflow from groundwater. Drainage through soil is also relevant, with nearly 900 t P y^{-1} infiltrating from landfills (33%), septic tanks (16%), and the rest as leaching from the nutrient present in the different land types considered in the MSA model, i.e. cropland, grassland, and forests. Table 4.7 reports 160 t P y^{-1} of atmospheric deposition, but contrary to N, the dominant contribution comes from wet deposition, 85%.

Similar to the analysis presented for N, values of intensive characteristics are compared to previous studies in Table 4.8, showing that results derived from the MSA simulation are more or less consistent with other studies (Antikainen, 2007; Kennedy *et al.*, 2007).

4.2.4 Carbon

The energy sector becomes the main actor of the carbon flows estimated by the model, as illustrated in Table 4.9. By far the largest C flux is the emission associated with transportation, which accounts for 57% of all emissions from local fuel consumption, which includes residential, commercial, industrial, and transportation, with a total of nearly 3.50×10^6 t C y^{-1}. Of the total emissions from transportation, 92% originates from gasoline combustion, and the remaining 8% from diesel and natural gas. The second flow responsible for local fuel

Table 4.7: List of the twenty most relevant phosphorus flows ranked by mass flow; the UCW in the year 2000.

Flow description[a]	**Mean value**[b] **($t\,P\,y^{-1}$)**	**Standard deviation ($t\,P\,y^{-1}$)**
Feed consumption by livestock	6287	467
Fresh manure generated	4086	777
Total nutrient applied to soil for fertilization	3637	392
Relevant material landfilled	3214	895
Total manure exported	(2470)	775
Food consumed	2116	202
Food produced	2023	70
Imports of Coal	+1940	1124
Coal Combustion Products	1940	1124
Total Treated Sewage Sludge Produced	1931	665
Inorganic Fertilizer imported/exported	+1317	78
Total soil infiltration	(899)	245
Total Imports of wood products	+615	46
Total Urine generated	486	123
Total Feaces generated	433	181
Recycled Paper	(390)	51
Leaching from landfills	(299)	80
Food waste generated	243	24
Total nutrient deposition	+157	37
Wastewater returns from WWTPs (effluent)	104	44

[a] NG: natural gas; PG: power generation; WWTP: wastewater treatment plant. For a complete list of abbreviations see Appendix A.

[b] Values in parenthesis are flows exiting the system, values preceded by the '+' symbol are entering the system, and the rest are internal flows of the system.

Table 4.8: Comparison of intensive system characteristics applied to phosphorus. All values reported on a per capita basis.

	MSA ($\mathbf{kg\,P\,y^{-1}}$)	**Other studies** ($\mathbf{kg\,P\,y^{-1}}$)
P in household wastewater	0.2–1.2	0.8^a, 0.6^b, 0.9^c
Municipal organic waste	0.15–0.22	0.20^a
Food consumption	1.3–1.9	1.1^a
Refuse food (as a percentage of consumed food)	8–17%	18%[a], 11%[b]
Use of fodder	4.0–5.5	3.0^b

[a] Source (Antikainen, 2007).
[b] Source (Schmid Neset *et al.*, 2008), scenario for year 2000.
[b] Source (Tangsubkul *et al.*, 2005).

emissions — non-power related — is generated by industrial operations amounting to about $1.17 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, or 32%. This leaves 8% for domestic and 3% for commercial fuel use. Biofuels in liquid form becomes relevant after the assumption that 10% of the gasoline and diesel for transportation is derived from organic sources. Power generation is responsible for the release of $1.24 \times 10^6\,\mathrm{t\,C\,y^{-1}}$; 95% of that comes from coal combustion while the rest is related to natural gas combustion. Almost 90% of the coal imported, $1.33 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, is for power generation and the rest is used for industrial purposes. Carbon in natural gas is imported at a rate of $7.13 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, mostly for non-power generation purposes (92%) including residential and commercial heating, industrial, and transportation.

Second in importance for carbon flows is the forestry sector, due to the large amount of carbon that is handled in wood material and forest floors. About 50% in the mass of wood products is carbon. The total imports of wood products represents about $0.92 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, and some 83% is supplied to the local market, while the rest is used for further processing by sawmills.

In the watershed context, hydrological processes have a a limited participation in C mobility, with riverine export being $65 \times 10^3\,\mathrm{t\,C\,y^{-1}}$ and atmospheric deposition $51 \times 10^3\,\mathrm{t\,C\,y^{-1}}$, 94% wet deposition, the most important in this group. The variability associated with deposition, represented by a standard deviation of about 50% of the mean value, is quite large, mainly because of the use of a lumped deposition rate for a region that has both rural and urban areas, and deposition decreases significantly as measurements are taken further from cities. See for instance (Lohse *et al.*, 2008) and (Kawamura *et al.*, 2001).

Metabolic respiration, including human and livestock, is probably an unexpected item in Table 4.9, but with $0.28 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, it has some significance in respect of the C fluxes of the overall system. Using Equation (3.20), C release as carbon dioxide is estimated to be $95\,\mathrm{kg\,C\,y^{-1}}$ per person, and for livestock, in 456, 5.3, and $124\,\mathrm{kg\,C\,y^{-1}}$ for cattle, poultry, and swine respectively. Human population and poultry account for 89% of the net respiration.

4.2.5 Energy

Environmental flows are the largest fluxes of energy into and out of the system. The net all-wave radiation (Q^*), $3.7 \times 10^6\,\mathrm{GWh\,y^{-1}}$, called here the effective solar energy input, is the major input to the system, see Equation (3.14). The total energy requirement of the system, $107\,000\,\mathrm{GWh\,y^{-1}}$ (all fuels and all purposes), is only 3% of the solar input. Most of this energy is lost via evaporation of water (Q_E), 55%, and the rest is distributed as turbulent sensible heat radiation $1.1 \times 10^6\,\mathrm{GWh\,y^{-1}}$ (Q_H) and storage heat flux (ΔQ_S) $0.6 \times 10^6\,\mathrm{GWh\,y^{-1}}$. The former represents the sensible heating of the air and the latter the heat accumulated in the surface, following different proportions for land and urban surfaces, both associated with the heat island phenomenon (Grimmond and Oke, 1986). More than 95% of the energy associated with water evaporation and transpiration comes from pervious areas and open

Table 4.9: List of the twenty most relevant carbon flows ranked by mass flow; the UCW in the year 2000.

Flow description[a]	**Mean value**[b] **(10^6 t C y^{-1})**	**Standard deviation (10^6 t C y^{-1})**
Emissions from local fuel consumption	(3.50)	0.26
Emissions from TR fuel use	(2.00)	0.23
Imports of coal	+1.33	0.13
Total emissions from PG	(1.24)	0.13
Emissions from IN fuel use	(1.10)	0.10
Total Imports of wood products	+0.92	0.06
Emissions from biomass use (non-power)	(0.71)	0.08
Imports of NG	+0.71	0.07
Imports of Biomass (for energy purposes)	+0.68	0.08
Carbon absorption during photosynthesis	0.63	0.10
Total feed consumption by livestock	0.36	0.03
Paper waste generated	0.36	0.03
Emissions from DO fuel use	(0.29)	0.03
Carbon Losses through metabolic respiration	(0.28)	0.01
Live trees removal	0.24	0.02
Relevant material landfilled	0.21	0.02
Imports/Exports of liquid biofuel	+0.20	0.02
Total food consumed	0.18	0.01
Recycled paper	(0.16)	0.02
Manure generated before losses	0.14	0.02

[a] NG: natural gas; PG: power generation; TR: transportation; DO: domestic. For a complete list of abbreviations see Appendix A.
[b] Values in parenthesis are flows exiting the system, values preceded by the '+' symbol are entering the system, and the rest are internal flows of the system.

water bodies, so that it is possible to assume that most of the accumulation of heat takes place in urban areas.

Over 53% of the total energy required by the system is supplied as eletricity, but only 6100 GWh y^{-1} are locally generated from power plants (84%) and by the two river dams in the Upper Chattahoochee River (16%). Local generation satisfies about 10% electricity required in the UCW. 90% of the energy content in imports of coal, 1.5×10^4 GWh y^{-1}, is used for power generation, while the rest is employed for industrial purposes. Gasoline is responsible of providing approximately 23% of the total energy required.

As for the assumption that water vapor (e.g. from evapotranspiration) is considered to have a latent heat value, some water flows are regarded to have a thermal energy value, if discharged at a temperature higher than the average temperature of the system. For example, 'Total water returned to surface sources', discharged from the WWTP and power generation plants, has an energy value of 5500 GWh y^{-1} due to its higher temperature relative to the average ambient temperature of 15°C.

The UCW relies to a great extent on fossil fuels, while the solar input seems to have the potential to provide much more energy than that required. Potentially, flows of returned water contain (mostly from power generation) enough energy to cover about 10% of the electricity demand of the UCW. In terms of energy associated with organic matter, animal feed and wood products are the most relevant. The portion of MSW considered in this study amounts to nearly 2900 GWh y^{-1}, but only 21% of the wood and food portion is assumed to be incinerated with an energy recovery of 150 GWh y^{-1}. Although the procedure does not reveal how feasible is the recovery of energy from the flows it gives a measure of the magnitude of energy contained in flows that might not be traditionally considered sources of energy.

Table 4.10: List of the twenty most relevant energy flows ranked by energy value; the UCW in the year 2000.

Flow description[a]	**Mean value**[b] **(10^3 GWh y^{-1})**	**Standard deviation (10^3 GWh y^{-1})**
Effective Solar Energy Input	+3733.1	300.6
Total water evaporation	(2038.8)	209.0
Turbulent sensible heat radiation	1103.4	193.5
Storage heat flux	595.5	289.9
Total Energy Required by the System (all uses)	107.0	4.2
Total electricity consumption	57.2	3.4
Imported/Exported Electricity	+51.2	3.4
Total gasoline consumption	24.7	2.2
Imports/Exports of Coal	+15.2	0.9
Imports/Exports of NG	+14.4	1.0
Total coal consumption for PG	13.6	1.0
Total natural gas consumption (non-power)	13.2	1.0
Emissions from coal PG	(12.7)	0.9
Total Imports of wood products	+10.0	0.7
Total biomass consumption (non-power)	8.1	0.7
Total soil infiltration	(6.7)	1.2
Total local electricity generation	6.1	0.3
Total water returned to surface sources	(5.5)	0.4
Total feed consumption by livestock	5.2	0.3
Relevant material landfilled	2.9	0.2

[a] NG: natural gas; PG: power generation; TR: transportation. For a complete list of abbreviations see Appendix A.
[b] Values in parenthesis are flows exiting the system, values preceded by the '+' symbol are entering the system, and the rest are internal flows of the system.

4.2.6 Aggregated Flows

Following the procedure described in Section 3.1.2, flows are aggregated into five categories: resources, products, air emissions, aquatic emissions, and solid wastes. This also makes possible estimating a term for the accumulation rate for each species, by using Equation (3.11). The resulting aggregated flows are presented in Figure 4.2, showing that for all species, excepting water, there is a positive accumulation. In the context of MSA, the flows under the label of *wastes* are materials sent for landfilling, regardless of the species. Consistent with other studies, e.g., Kaye *et al.* (2006); Tangsubkul *et al.* (2005), urban areas and human-managed watersheds (Jaworski *et al.*, 1992) behave as sinks of N and P. For instance, the UCW stored N and P at a rate of 19.6 and 3.7 $kg\,ha^{-1}\,y^{-1}$ respectively, which represents about 60% of the estimated values for the Potomac River Basin (Jaworski *et al.*, 1992). The Potomac Basin has 40% of its area dedicated to agriculture, compared to 10% for the UCW, suggesting that agriculture might play an important role in the accumulation of nutrients.

Water

Water in rural-suburban-urban systems is typically not accumulated (see Grimmond and Oke (1986)), as hydrological processes balance each other, and in the case of human-manipulated flows, most of the water withdrawn is returned to a water source.

Nitrogen

The major N inputs to the system are feed, fuels (coal and natural gas), and fertilizers, 90 000 $t\,N\,y^{-1}$, categorized as resources. Most of the fuel-bound N is release to the atmosphere, together with WWTP emissions and NH_3 volatilization from manure and fertilizers, 61 000 $t\,N\,y^{-1}$, but some input is received via deposition, 4300 $t\,N\,y^{-1}$. The major products are meat and poultry litter exported as a nutrient source, 11 000 $t\,N\,y^{-1}$. Most emissions to aquatic systems are the sum of the various sources of leachate and surface runoff from pervious and impervious areas (7700 $\mathrm{t\,N\,y^{-1}}$). The data suggest that accumulation is mostly related with the food sector, more specifically, fertilizers and animal feed.

Phosphorus

Phosphorus follows the case of nitrogen, in the sense that the food and energy sectors are the most relevant. P inputs can be identified as fodder import 6200 $\mathrm{t\,P\,y^{-1}}$, P in coal 2000 $\mathrm{t\,P\,y^{-1}}$, inorganic fertilizers 1300 $\mathrm{t\,P\,y^{-1}}$, and less so, imports of wood products 600 $\mathrm{t\,P\,y^{-1}}$. The input of P from deposition is the most import flow to and from the atmosphere 200 $\mathrm{t\,P\,y^{-1}}$. Aquatic emissions are for the most part contributions from surface runoff and soil infiltration, for a total of 2200 $\mathrm{t\,P\,y^{-1}}$. Discharges from WWTPs and other industrial operations are less significant. The main products containing P are manure and meat, 2500 $\mathrm{t\,P\,y^{-1}}$ and 900 $\mathrm{t\,P\,y^{-1}}$ respectively, making up 87% of all P in the system's products. Similar to N, it would be appropriate to say that the food sector is responsible for the accumulation of P.

Carbon

Carbon, on the other hand, is predominantly influenced by the energy sector. About 70% of the C that enters the system is lost as air emissions — unquestionably from fuel combustion. Roughly 92% of all the materials exported as products are recycled paper 164 000 $\mathrm{t\,C\,y^{-1}}$, wood products 88 000 $\mathrm{t\,C\,y^{-1}}$, and manure 73 000 $\mathrm{t\,C\,y^{-1}}$. Hence, in the case of C, there is a shift from only food and energy — observed for N and P — to energy and forestry. After losses to the atmosphere, hydrosphere, and lithosphere, 20% of the input C remains in the system. Because of the characteristics of the carbon cycle, the analysis for identifying the relevant causes of accumulation requires examination in detail of the nature of C inputs to the system. A large portion of the inputs is comprised of fossil fuels and biofuels (4 000 000 $\mathrm{t\,C\,y^{-1}}$), biomass (1 600 000 $\mathrm{t\,C\,y^{-1}}$), including 42% for fuel purposes, animal feed (350 000 $\mathrm{t\,C\,y^{-1}}$), and food (140 000 $\mathrm{t\,C\,y^{-1}}$). Carbon emissions from biomass used as fuel, 630 000 $\mathrm{t\,C\,y^{-1}}$, are almost compensated by the carbon sequestered by photosynthesis:

thus, the materials responsible for accumulation are mostly wood products, possibly associated with construction materials (Kennedy *et al.*, 2007), and to a lesser extent the manure generated from livestock operations.

Energy

In Section 3.3, Equation (3.14) is presented as a way to describe the solar energy that enters the system and the energy that can be accumulated in urban and land surfaces during daytime. The term of net heat storage, ΔQ_S, is reflected in the accumulation of energy shown in Figure 4.2, under ΔS, as if the city is continuously absorbing heat. However, as explained in Section 3.3, the term must be seen as a resource flow that is mostly available only during daytime (Grimmond and Oke, 2002), but which can be harvested by already-proven technologies (Mallick *et al.*, 2009), while most of it is lost during the night. Additionally, ΔS can be interpreted as a measure of the available heat that contributes to the urban heat island (UHI) effect, which has potential impacts on energy demand and air quality. Thus a system with a larger ΔS per unit of area has a larger potential for experiencing the UHI effect and exhibiting higher temperatures compared to neighboring rural areas. Metro Atlanta, for instance, has shown 5°C more than its surrounding areas (Dixon and Mote, 2003).

The flows identified as relevant to the aggregated flows for each species have better chances to be influential over the behavior of the indicators (see Section 3.1.2), as these measures are mathematically derived from the relationships among aggregated flows. The next Chapter is dedicated to expanding the *base case* presented here to a total of eight cases in an effort to explore the benefits of implementing three technologies (i.e. urine source separation, poultry litter pyrolysis, and municipal sludge pyrolysis) individually or in combination with the other two. The benefits or improvement are assessed on the basis of the performance of the whole system measured by the sustainability indicators.

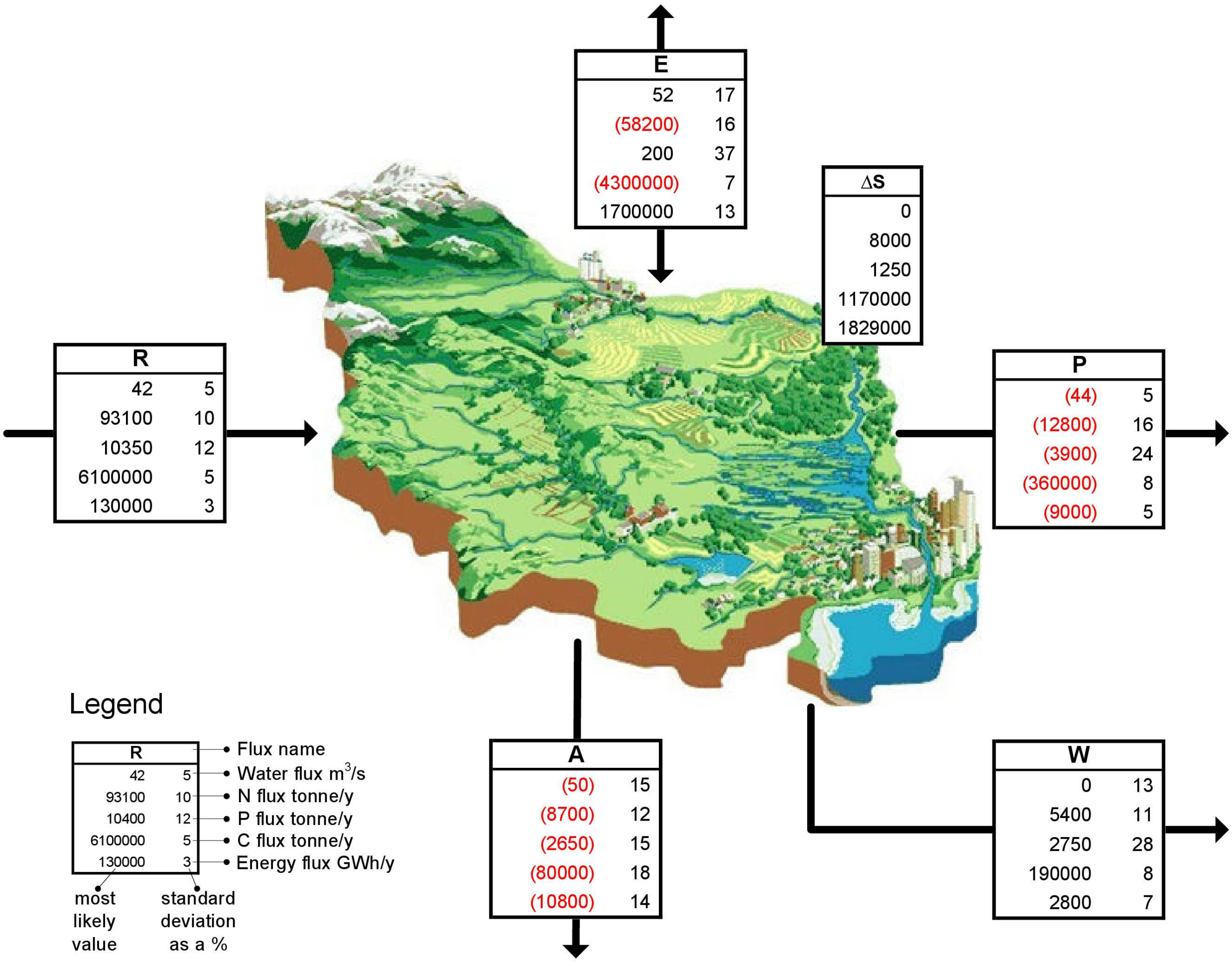

Figure 4.2: Aggregated flows of the UCW system (*base case*) after classified as resources (R), products (P), air emissions (E), aquatic emissions (A), and wastes (W); ΔS is the accumulation rate; values in red and parenthesis are outgoing fluxes, while black font color are inputs to the system. Image source: (AAFC, 2010).

Chapter 5

CASE STUDY PART II: Sustainability Assessment

"All truths are easy to understand once they are discovered; the point is to discover them." Galileo Galilei

This section takes advantage of the knowledge acquired about the system's behavior under normal operation — the *base case* in Chapter 4 — and proceeds to use the MSA to examine different combinations of scenarios created by the implementation of three relatively new technologies: source separation, poultry litter pyrolysis, and municipal sludge pyrolysis.

5.1 Exploring Structural Change

One of the objectives of the MSA framework is to have the capabilities for providing valuable information with regard to the potential effects that a *structural change* — also referred to herein as a technological innovation — can have in its own sector and on the rest of the industrial sectors. The selection of the three technologies mentioned before does not follow any particular interest but has instead been chosen to explore the modeling capacity of MSA for comparing scenarios and to assess their sustainability level. Of course, it is tempting to investigate regionally relevant and relatively new technologies, particularly those advertised as environmentally-friendly, with the hope of revealing added benefits — in addition to those already shown by previous studies — that would otherwise not be possible without a multi-sectoral view at a large scale, such as that of the UCW. Additionally, as in any data-intensive analysis, the availability of process information was a consideration on selecting the three candidate technologies.

5.1.1 Source separation

Source separation technologies, i.e., urine separation technology (UST), have been proposed as a solution for nutrient recovery in the water sector with possible implications for the reduction of nitrogen losses — as air emissions — from municipal wastewater treatment plants (WWTP) and fertilizer production. Source separation is a two-part story, first separating urine at the toilet level and, second, converting the recovered urine into a material (pharmaceutical- and hormone-free) with nutrient value (see for instance Larsen and Lienert (2007); Beck *et al.* (2010a)). The practical aspects of the implementation of the urine separation device (e.g., the NoMix toilet) and selecting either decentralized or centralized approaches for urine treatment has been subject to extensive investigation, e.g., Borsuk *et al.* (2008). There are also different processes by which urine is converted into a fertilizer such as biological stabilization, chemical precipitation, and physical separation using membrane technology (Larsen and Lienert, 2007). However, those details are not part of the scope of this dissertation. Urine treatment is considered therefore as a black box with the process characteristics of a chemical precipitation unit that generates two products: struvite $MgNH_4PO_4 \cdot 6(H_2O)$, and ammonium sulphate $(NH_4)SO_4$ at a certain efficiency rate (Beck *et al.*, 2010a). Struvite is produced at a rate according to the availability of P in urine — typically the limiting nutrient — and the remaining N is synthesized as $(NH_4)SO_4$. The formation of struvite has been already studied due to its accidental formation, and the operational upsets that this involves, in WWTP pipelines (Doyle and Parsons, 2002). Moreover, struvite is considered a valuable slow-release inorganic fertilizer with important economic advantages given the fact that it is being produced from flows regarded as waste (Shu *et al.*, 2006).

5.1.2 Pyrolysis: Poultry litter and municipal sludge

As a complement to the decentralized nature of urine separation, i.e. on a household basis, pyrolysis is introduced as a centralized application for both rural (poultry) and urban (municipal sludge) situations. Corroborated in terms of nutrients in respect of the *base case*, the economic relevance of the poultry industry in the UCW is well known; therefore, it makes sense to incorporate in the MSA the poultry litter pyrolysis process, technology that is also being studied at the University of Georgia (Das *et al.*, 2008), making data more accessible. In general terms, the pyrolysis process is capable of breaking organic material into liquid, solid, and gaseous products. The yield of each phase, and its composition, varies not only with the material fed but also with the operating conditions, i.e. heating rates and final temperature. Slow heating rates produce more char, while high heating yields more gas and liquids (Onay and Kockar, 2003). Typically, the liquid and the gaseous phase are considered for fuel purposes, while the solid phase, also called *char*, is usually regarded as a nutrient source. The calculation of the flows of N, P, and C in the products of the pyrolysis process starts with the estimation of partition coefficients based on reaction kinetics, for which the MSA assumes a one-stage mechanism with parallel reactions for each species following the Arrhenius equation, see Equation (5.1). Di Blasi and Branca (2001), and originally Shafizadeh and Chin (1977), use this approach for the estimation of reaction rate constants, under isothermal conditions, and then calculate a yield coefficient of each phase produced from the pyrolysis of wood material as follows,

$$k_j = A_j \cdot e^{\left(\frac{-E_j}{R \cdot T}\right)} \tag{5.1}$$

where k_j is the kinetic or reaction rate constant for the jth phase (liquid L, solid S, and gas G) in s^{-1}; A_j is a pre-exponential constant in s^{-1}; R is the universal gas constant ($8.31 \times 10^{-3}\,\mathrm{kJ\,mol^{-1}\,K^{-1}}$); T is the reaction temperature (K); and E_j is the activation energy of reaction ($\mathrm{kJ\,mol^{-1}}$). With this, a global reaction rate can be calculated,

$$k_{global} = k_L + k_S + k_G \tag{5.2}$$

where k_{global} is the global reaction rate, and k_L, k_S, and k_G are the kinetic constants for the rates of product formation for liquid, solid, and gas respectively. The yield of each product can be expressed as,

$$Y_L = \frac{k_L}{k_{global}}$$

$$Y_S = \frac{k_S}{k_{global}} \tag{5.3}$$

$$Y_G = \frac{k_G}{k_{global}}$$

where Y_L, Y_S, and Y_G are the yield coefficients for liquid, solid, and gas respectively. However, besides the availability of calculating mass distribution among pyrolysis products, it is necessary also to calculate the portion of N, C, and P that remains in each product, i.e. liquid, gas, char. In the case of phosphorus, it is assumed that 100% of the amount fed to the process is recovered in the solid phase. On many occasions, biomass pyrolysis has been approached under the assumption that the main components of biomass (cellulose, hemicellulose, and lignin) behave independently during the pyrolysis process (Chen *et al.*, 1997). This approach is extrapolated to the behavior of carbon and nitrogen, and empirical yield coefficients for mass and nutrients are calculated based on data generated by Sánchez *et al.* (2007); Das *et al.* (2008); Singh (2008); Zhang *et al.* (2009b); Di Blasi and Branca (2001). Considering a reaction temperature of 500 °C, the values of specific activation energies E_j can be estimated by simultaneously solving Equations (5.3), (5.2), and (5.1), while handling the pre-exponential term for the corresponding product phase A_j as a constant for all species. Table 5.1 presents the activation energy and constants used for the estimation of the pyrolysis products and its composition.

Table 5.1: Estimated kinetic constants for sludge and manure pyrolysis.

		Activation Energy, E (kJ mol^{-1})	**Pre-exponential constant, ln$A$**
Liquid, k_L	for N	158	23.1
	for C	163	
	total phase	168	
	total phase (wood)[a]	148	
Solid, k_S	for N	114	15.0
	for C	111	
	total phase	113	
	total phase (wood)[a]	112	
Gas, k_G	for N	164	22.2
	for C	161	
	total phase	160	
	total phase (wood)[a]	153	

[a] Phase yield coefficient estimated by (Di Blasi and Branca, 2001); presented for comparison purposes.

The energy content of each product is estimated using the equation proposed by Channiwala and Parikh (2002) for liquid, gaseous, and solid fuels, but additionally, the distribution of energy must comply with the energy balance applied to the pyrolysis process as a whole, used by Raveendran and Ganesh (1996) for various types of biomass,

$$H_B = H_L \cdot Y_L + H_S \cdot Y_S + H_G \cdot Y_G \tag{5.4}$$

where H_B, H_L, H_S, and H_G are the energy content of the pyrolysis feed flow, and its products, liquid, solid, and gas respectively.

5.2 Sustainability Performance

Seven cases can be specified by the combination of the technologies of urine seperation (UST), poultry litter pyrolysis (PLP), and municipal sludge pyrolysis (MSP), each alternating in a binary fashion between 0% and 100% of implementation (See Table 5.2). The degree of implementation for UST, parameter α_{98}, is defined by the fraction of the population using this technology. In the case of PLP and MSP, parameters α_{193} and α_{195} respectively, the degree of technology usage is reflected in the fraction of mass of poultry litter and treated municipal sludge sent to the pyrolysis process. Together with the *base case* (described in Chapter 4), a total of eight scenarios are considered for this study case.

Table 5.2: Scenario definition through various combinations of technology implementation parameters, where 0 is 0% implementation and 1 is 100% implementation.

Scenario code	**Parameter values**		
	α_{98} (UST)	α_{195} (MSP)	α_{193} (PLP)
R000	0	0	0
R100	1	0	0
R010	0	1	0
R001	0	0	1
R110	1	1	0
R111	1	1	1
R101	1	0	1
R011	0	1	1

The generation of scenario results uses the same parameter vector sampled with the Monte Carlo simulation for the *base case* so that only change introduced is derived from the adjustments of the parameters described in Table 5.2. Results, material and energy flows, are then used to calculate the values of sustainability indicators as described in Section 3.1.2 (also refer to Table 3.2 for nomenclature and definition of the indicators). The first four measures (indicators PRI, RWI, PWI, and EEI) make possible the comparison of scenarios based on their efficiency and eco-efficiency. The remaining four (indicators HAE, HWE, WEF, and E2I) compare the performance of the system versus a reference state characterized as, for the purposes of this case study, an undisturbed forest with the terrain and climatic conditions of the Upper Chattahoochee Watershed. This pre-industrial state corresponds to those non-human flows that would take place in a fully forested watershed and upon which the healthy emissions to air, E_k^0, and to water, A_k^0, are estimated. The first includes processes such as denitrification, N fixation, deposition (wet and dry), C absorption via photosynthesis, and C release via respiration. The second is simply the losses of N, P, and C via surface runoff and soil infiltration. More details on these processes can be found in Section 2.3. For the specific case of the Upper Chattahoochee Watershed, the calculated values for E_k^0 and A_k^0, presented in Table 5.3, are assumed to provide a sustainable level of ecosystem services, e.g. adequate nutrients for aquatic biota. Because the reference state (the undisturbed forest) is based on field measurements and limited knowledge of what this pre-industrial state would have been, its definition also accounts for the uncertainty of the atmospheric and hydrological processes involved, as described by the standard deviation reported in Table 5.3.

5.3 Results and Discussion

The simulation-generated data for the eight scenarios are condensed into Figures 5.1, 5.2, 5.3, 5.4, and 5.5. The line plot represents the mean value obtained for indicators while the bars indicate the maximum and minimum values within a 95% confidence interval. When analyzing these plots, it is important to remember that the objective of the upper four graphs is to maximize their value, while for the remaining four the desirable value is unity, shown as a red line if the scale of the plot permits its visualization.

Table 5.3: Estimated healthy emissions for the reference state, the undisturbed forest. These values are used for the calculation of indicators HAE, HWE, and WEF.

Emission type	**Species**[a]	**Mean value**[b]	**Standard deviation**
Atmospheric (E_k^0)	Water ($\times 10^6$)	1430	292
	N	(763)	1494
	P	134	65
	C ($\times 10^6$)	3.5	2
	Energy ($\times 10^6$)	1.6	0.2
Aquatic (A_k^0)	Water ($\times 10^6$)	(1430)	292
	N	(16490)	3531
	P	(1982)	732
	C ($\times 10^3$)	(109.7)	23
	Energy ($\times 10^3$)	(8.3)	1.7

[a] All units in tonnes per year, excepting for energy, in which case, GWh y^{-1} applies.
[b] Values in parenthesis are flows exiting the system.

5.3.1 Water

The most straightforward benefit at the household level is the water savings introduced by the UST in scenarios R100, R110, R111, and R101. On average, it results in a reduction of domestic water use of 7% at a volume rate of $0.35\,\mathrm{m^3\,s^{-1}}$, enough to fill 4400 Olympic swimming pools. However, this is barely comparable to other flows such as total water withdrawals, $42\,\mathrm{m^3\,s^{-1}}$. In Figure 5.1, the effect of UST at the watershed level is hardly noticeable for the same reason, the large magnitude of other flows that is.

The mean value of indicators RWI and PWI improved 35% compared to the *base case* with the implementation of sludge pyrolysis, scenarios R010, R110, R111, and R011. These two indicators are very sensitive to the flow of water in municipal solid waste (MSW), which is reduced by the diversion of sludge to the pyrolysis process. Besides RWI, and PWI, all indicators remain essentially constant. PRI, for instance, ranges from 1.01 to 1.08 which means that the system delivers 1–8% more water than the amount withdrawn. This increment is probably due to the incorporation of rainfall water into the sewer network (via inflow and infiltration). Similarly, WEF acknowledges this excess of water in the *product* flows, driving the indicator 0–12% above the desired level. HWE suggests that surface runoff is 0–25% larger than the value calculated for the reference state, while HAE shows that water is evaporated at a rate 5–25% higher. Under certain conditions, these three indicators (WEF, HAE, and HWE) reflect that the system is not too far from the hydraulic characteristics of the reference state, possibly because 90% of the watershed is pervious surface, of which about 56% is forested land.

5.3.2 Nitrogen

Although the first four plots (efficiency and eco-efficiency) seem to exhibit exactly the same trend, there is some information that can be drawn at first sight from these plots (see Figure 5.2). The plots for PRI and EEI are quite similar excepting their magnitude, suggesting

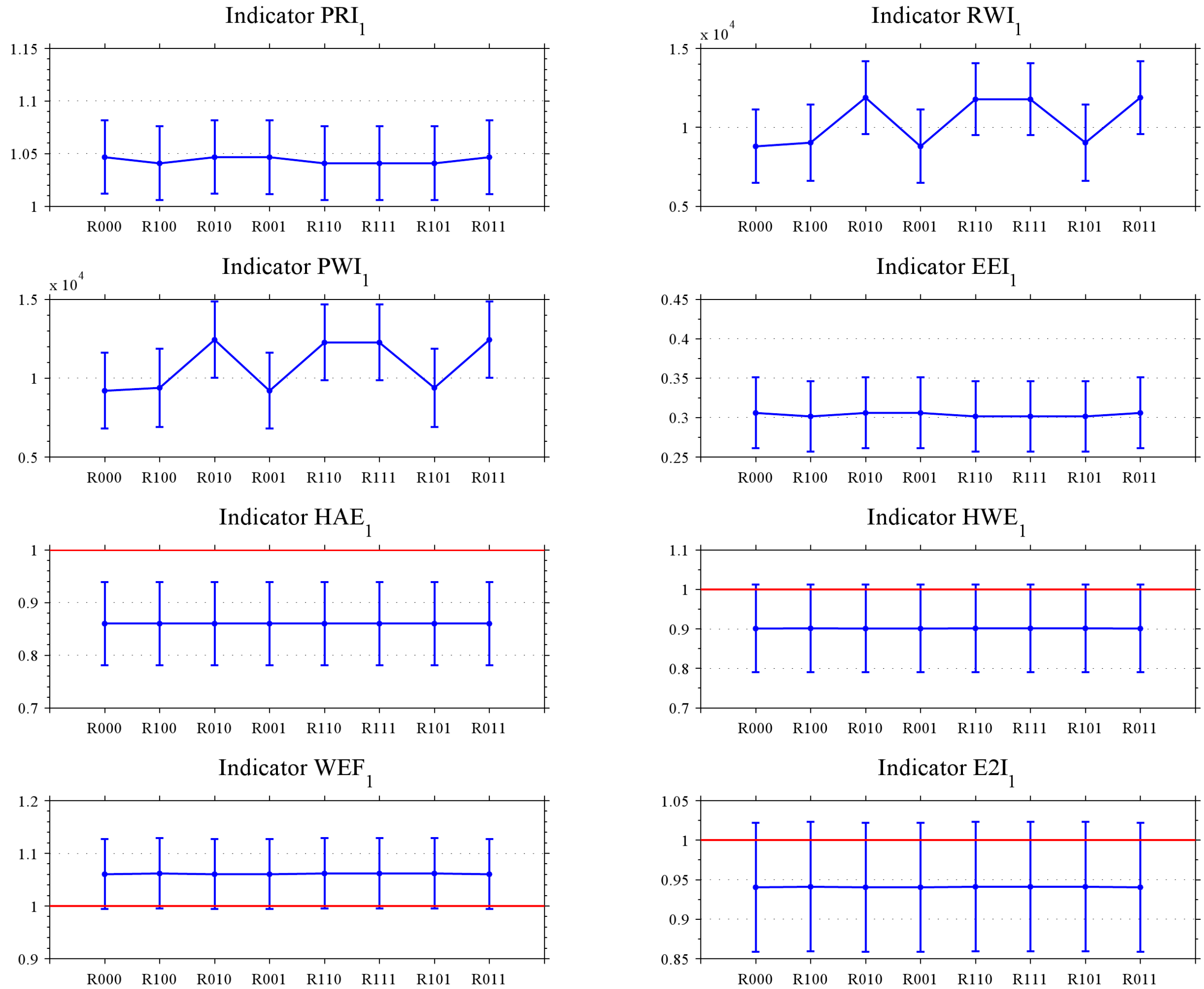

Figure 5.1: Performance of indicators for water. Each plot represents the performance of an indicator (as labeled), under eight different scenarios, ordered from left to right: R000, R100, R010, R001, R110, R111, R101, R011. The red line, unity, is the desirable value for the lower four plots.

that about 85% of the resources are lost as emissions to the atmosphere and water bodies. PRI ranges from 0.1 to 0.2 suggesting that only 10–20% of the resources received by the UCW are returned to other systems in the form of a *product*. The amount of N wasted is small compared to the resources consumed (4–8%), but it is relatively large compared to the products generated (25–75%). HAE shows that air emissions are much higher than those defined for the reference state (undisturbed forest), while emissions to aquatic systems via runoff and infiltration can be 60% lower. The former is due to the large component of fuel N in air emissions, lowering the eco-efficiency of the system (EEI_2) to a 10–23% range.

The best improvement in terms of N appears to be introduced by UST and MSP together, but mainly due to MSP. If municipal sludge is fed to the pyrolysis process, about $900\,\mathrm{t\,N\,y^{-1}}$ are recovered as a fuel and fertilizer instead of being sent to landfill, which improves notably the mean value of PWI_2 by some 22%, and RWI_2 by 16%. Although represented by a much larger flow that spares the need for inorganic fertilizer by $4000\,\mathrm{t\,N\,y^{-1}}$ or almost 45% of the total consumption of fertilizer, UST has marginal influence on all indicators, suggesting that even though it appears to be important at the household level (see Section 4.2.2), at the watershed level it is less significant. The explanation is also related to the structure of the indicators that seem to penalize more the generation of waste (represented by a single flow) than the reduction of resource requirements, which is a highly aggregated flow. However, UST reduces N air emission and effluent load at WWTPs by almost 40%, down to 3500 and $950\,\mathrm{t\,N\,y^{-1}}$ respectively, contributing to the slight improvement of HAE (air emissions) and HWE (discharges to water bodies), but it has not a noticeable impact because of the large magnitude of N in air emission from fuel combustion, also part of indicators EEI_2, HAE_2, WEF_2, and $E2I_2$. The nitrogen content in municipal sludge is also reduced by 18%, sending $150\,\mathrm{t\,N\,y^{-1}}$ less to landfills. If MSP is implemented together with UST, a total of $750\,\mathrm{t\,N\,y^{-1}}$ is spared from landfills, which consequently reduces the amount of N leached by almost 15%, from $950\,\mathrm{t\,N\,y^{-1}}$ to $820\,\mathrm{t\,N\,y^{-1}}$, hence also improving HWE_2. By implementing the three technologies at the same time, a total of $9250\,\mathrm{t\,N\,y^{-1}}$ is recovered in the form of fuels (46%), and as fertilizer (54%).

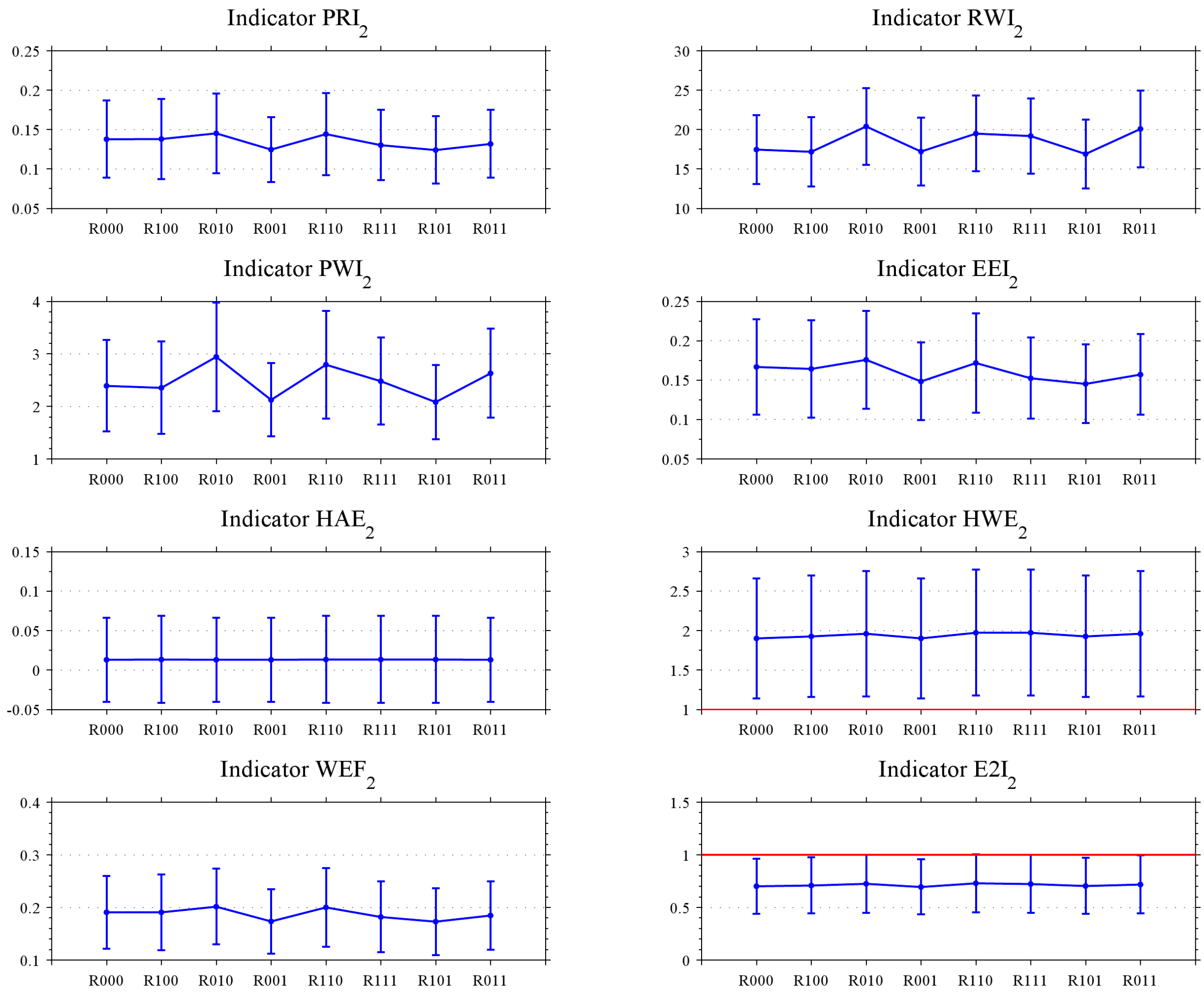

Figure 5.2: Performance of indicators for nitrogen. Each plot represents the performance of an indicator (as labeled), under eight different scenarios, ordered from left to right: R000, R100, R010, R001, R110, R111, R101, R011. The red line, unity, is the desirable value for the lower four plots.

Besides MSP, the $4500\,\mathrm{t\,N\,y^{-1}}$ sent for poultry litter pyrolysis appears as a big influence for most of the indicators. For the first four indicators, PLP seems to have a negative effect mainly because the model considers export manure a *product*, which results in a more influential flow, in terms of N, than the separated benefits that pyrolysis has in terms of energy and fertilizer production. For instance, by utilizing the products derived from pyrolysis for energy purposes, the N associated with poultry litter exits the system as an emission, and is therefore accounted for differently. The reaction of indicator WEF is clearly correlated to PRI, which is logical if the accumulation of material and the healthy emissions to air and water remain constant. However, WEF provides extra information by comparing the actual amount of *product* from the system to the value of the reference state, where all resources are used in a sustainable manner. Additional to the marginal improvement of 5% in terms of the mean when sludge pyrolysis is implemented, WEF indicates that the system is about 80% less productive than an undisturbed forest, or if interpreted inversely, a larger proportion of the resources left after satisfying the internal need for resources (described by the accumulation) and a level of healthy emissions is not used to generate a useful flow. For all scenarios, the weighting parameters of Equation (3.12), are assumed to have the same importance, that is $\beta_{1,k} = \beta_{2,k} = \beta_{3,k} = 1/3$, so the large magnitude of HWE compensates for the lower scores of HAE and WEF and moves E2I towards unity, without actually meeting all three eco-effectiveness criteria. This means that the four indicators associated with eco-effectiveness have to be analyzed together in order to generate solid conclusions.

5.3.3 Phosphorus

In general, Figure 5.3 shows that the variability of the indicators applied to P is much larger than that of nitrogen. For instance, PRI_2 (nitrogen) varies from 0.1 to 0.2 (a $\times 2$ factor), but PRI_3 (phosphorus) displays a range 0.2–0.6, with larger magnitude and a $\times 3$ factor. Similarly, RWI_2 varies over a range of about 13 to 25 (again $\times 2$ factor) while RWI_3 values are lower but with a larger proportional variation, 2.0–10 or a $\times 5$ factor. This implies that the information provided to the model with respect to P, in the form of parameters and input data, bares more uncertainty compared to Nitrogen.

Given that P is not lost to the atmosphere but reconcentrated in municipal sludge, UST has a larger effect on the P present in sludge, compared to nitrogen, by reducing its content in about 25% or from $1200\,\mathrm{t\,P\,y^{-1}}$ to $900\,\mathrm{t\,P\,y^{-1}}$. Implementing MSP prevents landfilling of the remaining P in sludge, resulting in a total reduction of 40% of the P in leachate. Phosphorus recovery from urine is $390\,\mathrm{t\,P\,y^{-1}}$, which is capable of supplying a third of the inorganic fertilizer P required in the region. During pyrolysis, almost 100% of the sludge P is recovered in the solid phase, contrary to N where some is lost to the gas and liquid phases; therefore, implementing MSP increases in such a way the production of P fertilizer that most of the UCW requirement is satisfied. The previous analysis explains the significance of UST and MSP for the performance of the indicators. Those scenarios where MSP is implemented (especially R010, R110, R111, and R011) show the best performance for most indicators with an improvement of the mean value on the order of 16% for PRI, 50% for RWI, 70% in the case of PWI, and more than 20% for EEI. Similar to N, removing poultry litter (using PLP) from the flow of *products* has a negative effect on those indicators that involve the P_k flow. However, its influence is less dramatic than for N, due to the importance of MSP in terms of P. For instance, compare the slope of PRI, for N and P, around the R111 scenario.

HAE is not modified by the inclusion of any of the technologies, thus its distance from the desired value (unity) is simply the presence of particulate P in coal and MSW combustion emissions. Consequently, P emissions to air are in much better shape compared to N with respect to the reference state. On the other hand, HWE is consistently improved by MSP, and to a less extent by UST, while PLP has no influence at all. In more detail, when HWE_3 (phosphorus) is compared with HWE_2 (nitrogen), it is found that aquatic emissions for P are larger than the desired level, but for N these are smaller. With no intentions of discussing about which nutrient is limiting to processes such as eutrophication, the analysis reveals that non-point sources of P should be reduced, while N releases might not be enough to satisfy ecosystem needs. The importance of P for eutrophication in Georgia, US, and particularly in the Piedmont area is well documented by previous studies, e.g. (Romeis and Jackson, 2005; Byers *et al.*, 2005; Zeng *et al.*, 2006)

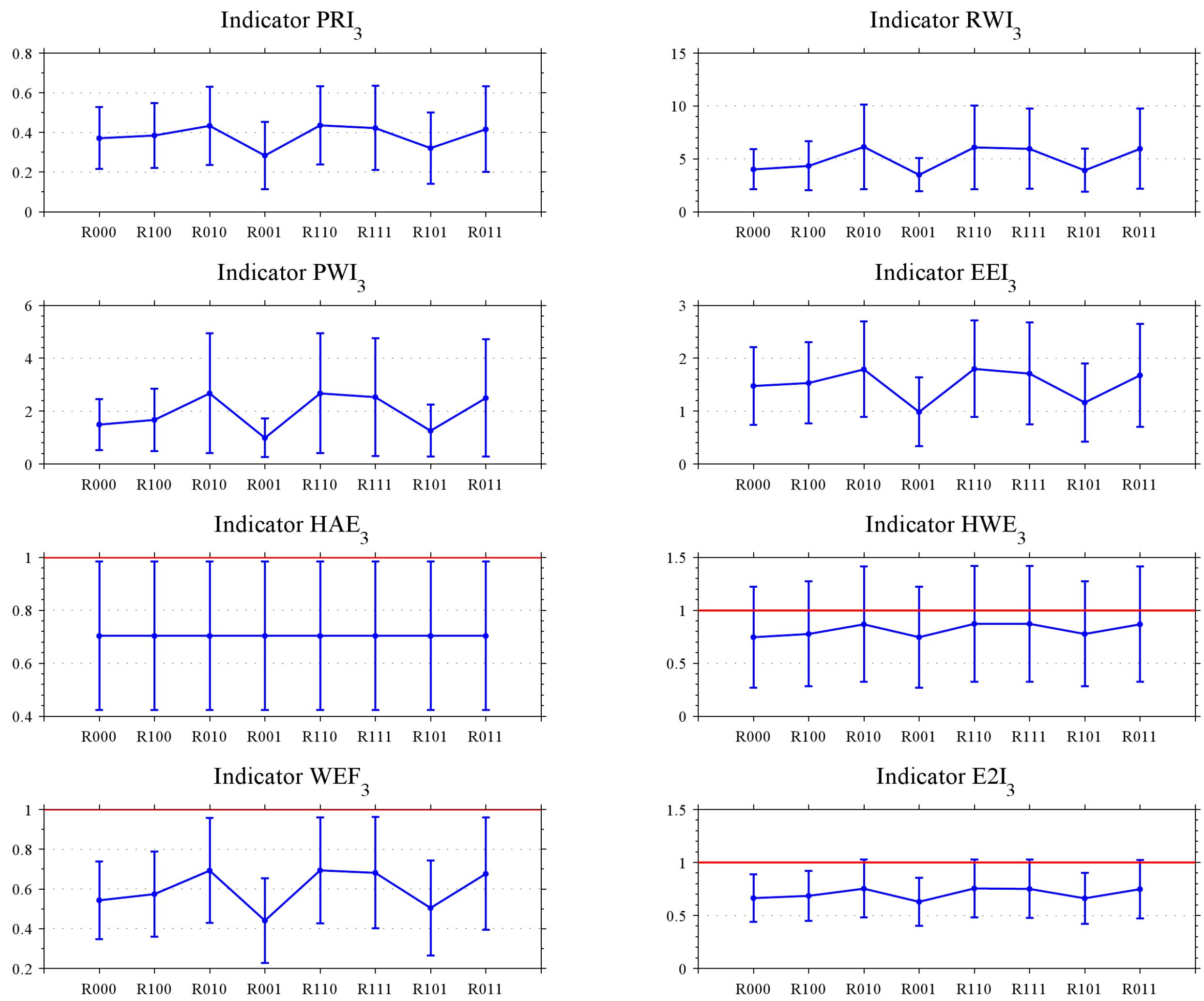

Figure 5.3: Performance of indicators for phosphorus. Each plot represents the performance of an indicator (as labeled), under eight different scenarios, ordered from left to right: R000, R100, R010, R001, R110, R111, R101, R011. The red line, unity, is the desirable value for the lower four plots.

WEF suggests that the system's productivity is more effective in terms of P than N, with a 20–60% score in the worst scenarios, but 40–100% when MSP is implemented. The best score for N in any scenario is about 27%. This is probably due to the active participation of N in atmospheric processes via air emissions, with thus less remaining in products. The aggregation of indicators HAE, HWE, and WEF define E2I, which shows little variation among scenarios and scoring 40–100%. The high score of E2I is mainly driven by those conditions under which HWE is higher than one, which means that the load of P in aquatic emissions is lower that the defined healthy P emission.

5.3.4 Carbon and Energy

After the analysis of flows in Chapter 4, there are little expectations of improvement for carbon as the technologies selected do not manipulate the most important flows associated with carbon and energy, Figures 5.4 and 5.5 respectively. The slight variation shown by indicators PRI, RWI, PWI, EEI, and WEF, is due to the material that is being spared from landfilling by the implementation of MSP. However, the values of the indicators (as shown for other species) provide information of the overall performance on the UCW.

Carbon

In the case of undisturbed forests, and assuming that no fire is taking place, the net flux of carbon is always from the atmosphere to the system (a positive flow for the effects of MSA), while in the UCW case, it is found that the carbon flux is always negative (outbound flow), as described by HWE_4 (carbon). About 50–80% of the carbon in the *resources* flows is lost as an atmospheric emission. The magnitude of C emissions varies from 50% to 9 times of the flux of the reference state, but in the opposite direction. C losses via runoff and infiltration are shown to be usually less than that of a forest, on occasion half of this value, as carbon release depends to a significant extent on the C content in the floor organic layer. Similarly to other species, WEF has the same trend displayed by PRI, but this time WEF is mostly less than PRI. The reason for this is that the healthy emissions of C are expected to be positive, thus more C is available for generating the adequate amount of *products*, in terms of eco-effectiveness, and therefore lowering the vertical axis of WEF.

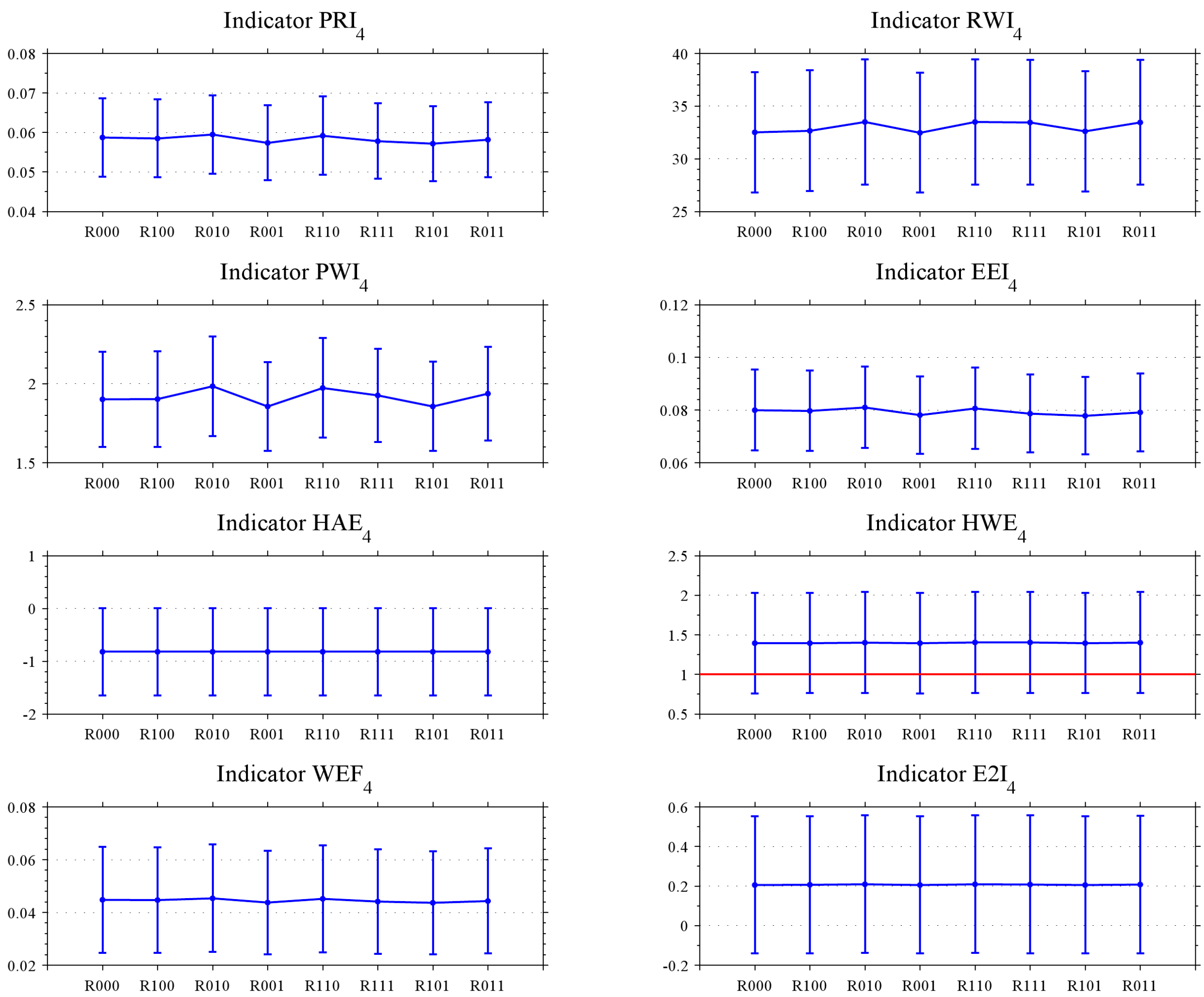

Figure 5.4: Performance of indicators for carbon. Each plot represents the performance of an indicator (as labeled), under eight different scenarios, ordered from left to right: R000, R100, R010, R001, R110, R111, R101, R011. The red line, unity, is the desirable value for the lower four plots.

Energy

Since most of the exported products are related with the food and forestry industries, and no energy is exported, a low score for PRI_5 (energy) and WEF_5 is expected. Only 6–8% of the energy contained in *resources* flows is returned as *products*. In the context of MSA, the system tends to accumulate part of the energy received via solar radiation (see explanation in Section 4.2.6), and if this accumulation plus the net income solar radiation is larger than the flow of *resources* and the losses via evaporation of water, then negative values of WEF_5 can take place, as it is the case in Figure 5.5. As WEF moves below unity, and even more if below-zero values are obtained, there is more energy available (captured initially as surface heating) waiting to be converted into an useful flow.

Indicator EEI has an extremely low magnitude compared to other species because radiation fluxes (including from the sun) are considered are part of the *emissions* term. As expected, the thermal energy in aquatic emissions from the UCW is 10–55% higher than the one a forest is supposed to release.

5.3.5 Additional Remarks

Aggregated flows

To complement the analysis presented in this chapter, Figure 5.6 shows the values of aggregated flows for scenario R111 (all technologies implemented simultaneously). Most of the changes take place for N and P. The need for resources is reduced by 6% and 13% for N and P respectively. Nitrogen emissions are reduced by only 3%, since most of the emissions are released from fuel combustion. The interesting point is that all flows of nitrogen decreased in their magnitude; assuming that economic activity within the region has not changed significantly, i.e., that consumption and waste generation remains the same, this can only suggest that the implementation of UST, MSP, and PLP, together, has a positive influence over the circularity of the nitrogen metabolism within the UCW. This is corroborated by the slight improvement shown by indicator E2I after comparing R000 and R111 for nitrogen. In the case of P, the shift from the *base case* to the R111 scenario is clearly reflected in the increased accumulation of P within the soil. Less P is sent as a product by diverting the poultry litter

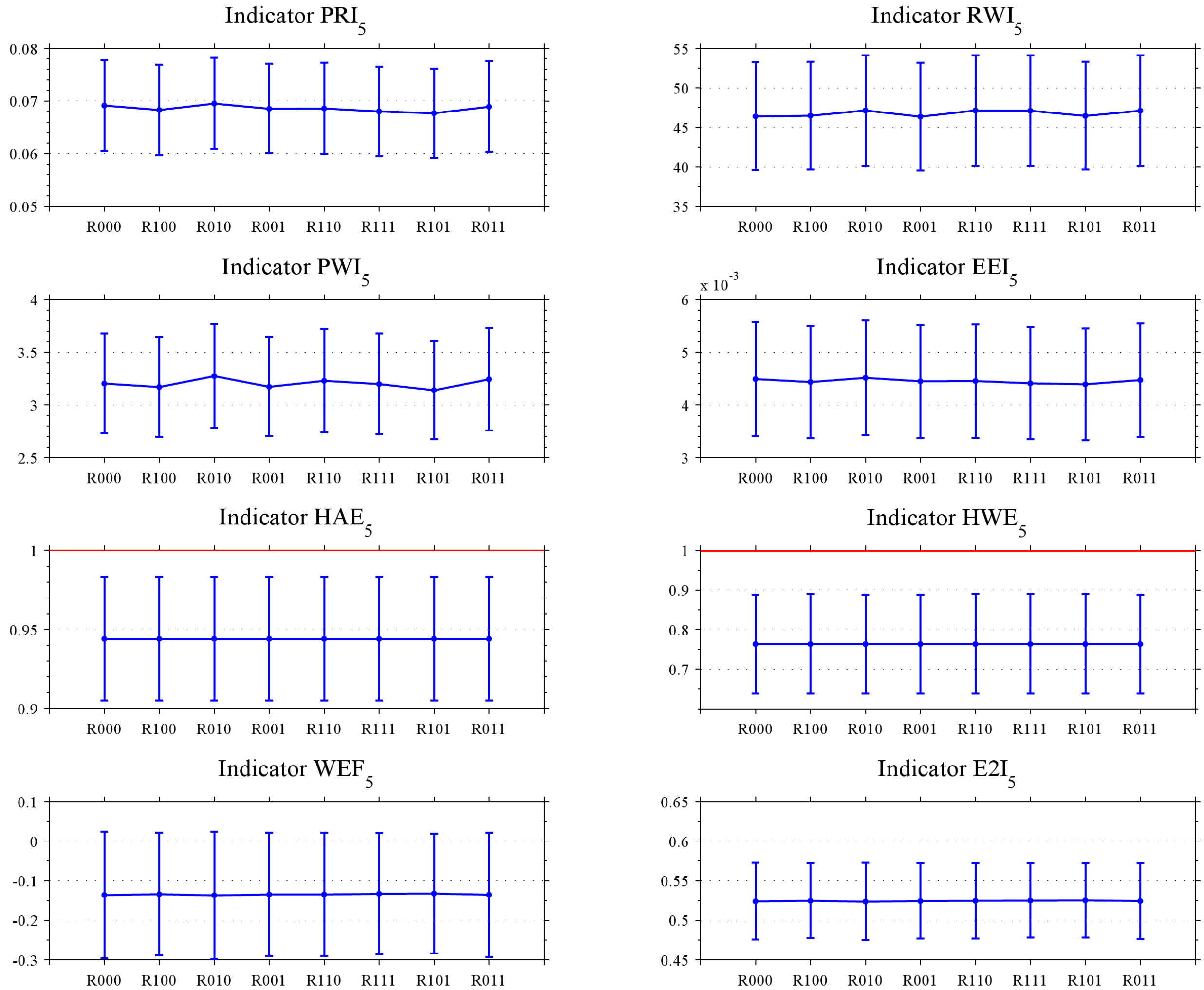

Figure 5.5: Performance of indicators for energy. Each plot represents the performance of an indicator (as labeled), under eight different scenarios, ordered from left to right: R000, R100, R010, R001, R110, R111, R101, R011. The red line, unity, is the desirable value for the lower four plots.

flow to the pyrolysis process, and less P is lost via leaching from landfills, thanks to the implementation of UST and MSP.

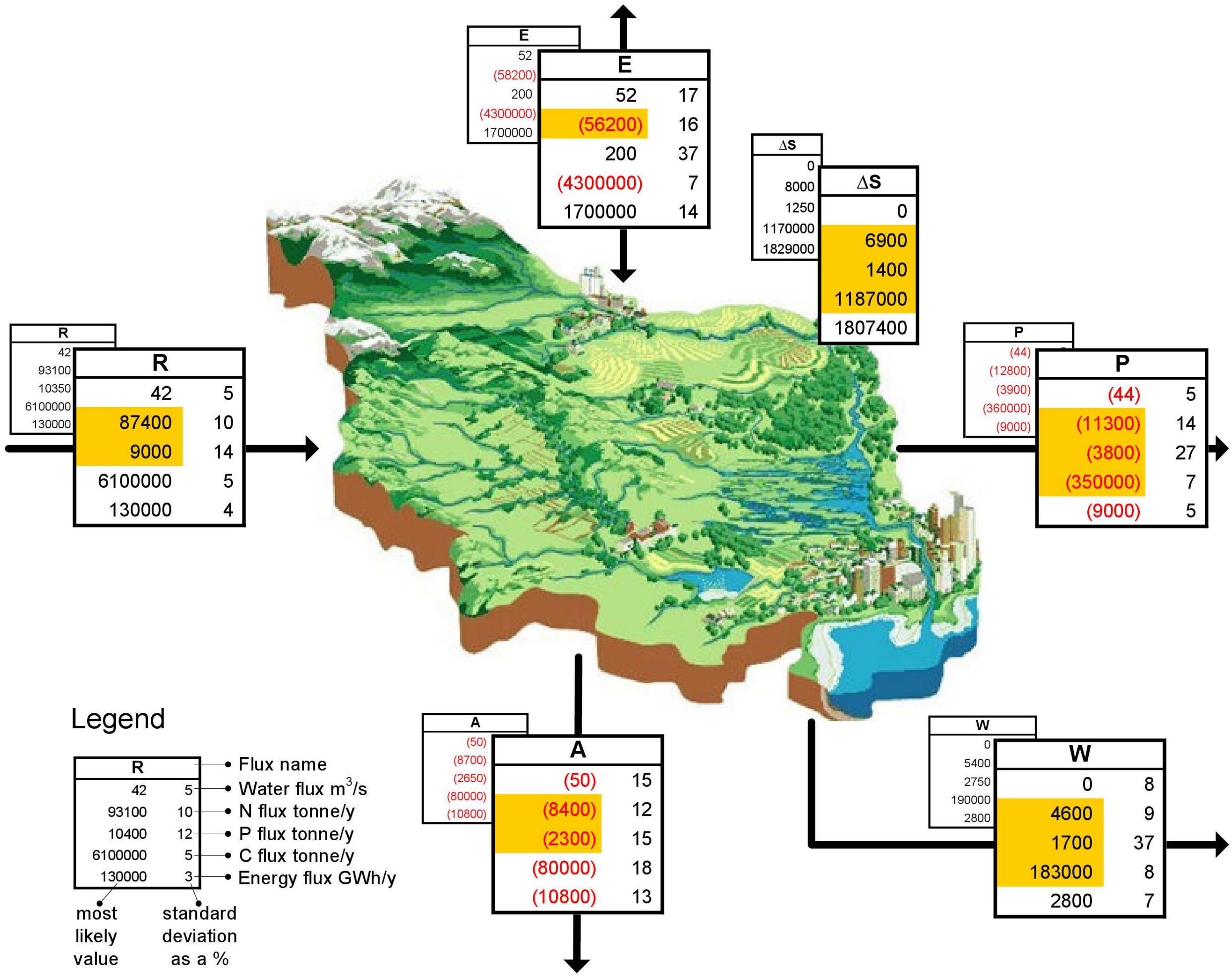

Figure 5.6: Aggregated flows of the UCW system after classified as resources (R), products (P), air emissions (E), aquatic emissions (A), and wastes (W); ΔS is the accumulation rate; values in red and parenthesis are outgoing fluxes, while black font color are inputs to the system. For comparison, small boxes show values corresponding to the *base case*, while large boxes show scenario R111 with highlighted values to indicate that a change in magnitude has occurred with respect to the *base case*. Image source: (AAFC, 2010).

Testing MSA for Carbon and Energy

In the detailed analysis for carbon and energy, in Section 5.3.4, it was found that the three technological solutions have moderate to important effects over the food sector, but little effect on the energy sector, hence on carbon flows. As a means to test, and illustrate, the capabilities of MSA for assessing energy and carbon aspects, two additional scenarios are briefly introduced herein. These scenarios, called for identification purposes *pseudo* 1 and 2, modify two of the major flows identified in Chapter 4:

(a) *Total Emissions from Power Generation*, scenario P–1. Imagine there is a way to sequester 50% of the emissions generated in UCW power plants, and convert the nutrients contained in those emissions into a *product*.

(b) *Storage heat flux*, scenario P–2. What would be the benefit of converting 10% of the heat flux accumulated on the watershed surface (e.g. land, buildings, roads) into electricity?

These two *pseudo* scenarios are described by the indicators behavior exhibited in Figures 5.7 and 5.8 for scenario P–1, and Figure 5.9 for scenario P–2. The sequestration of power generation emissions (P–1) results in an increased productivity in terms of N (Figure 5.7), acknowledged by PRI, PWI, and WEF. The eco-efficiency indicator (EEI) also improves, but for two reasons, increased N in *products* and reduced N in emissions to air. Despite the decrease in air emissions, the effect on HAE is less noticeable. The improvement of E2I is slightly more evident than the rest of the scenarios. The performance with respect to C (Figure 5.8), is also substantially better. A curious point is the apparent worsening shown by HAE, a situation that is reflected in E2I; However, HAE is actually improving. Figure E.1 in Appendix E shows that for the particular case of C, for which a positive flux of carbon is desirable, in order to reach the $\mathrm{HAE}_4 = 1$ point, a negative flux moving towards A_4^0 decreases the value of HAE.

Several things can be said about scenario P–2. First, it has no relevance for air and aquatic emissions. Second, it shows noticeable changes with respect to other scenarios but with a great level of uncertainty. This might suggest that energy from solar radiation can bring large amounts of benefits but is not reliable enough to be considered as a straightforward

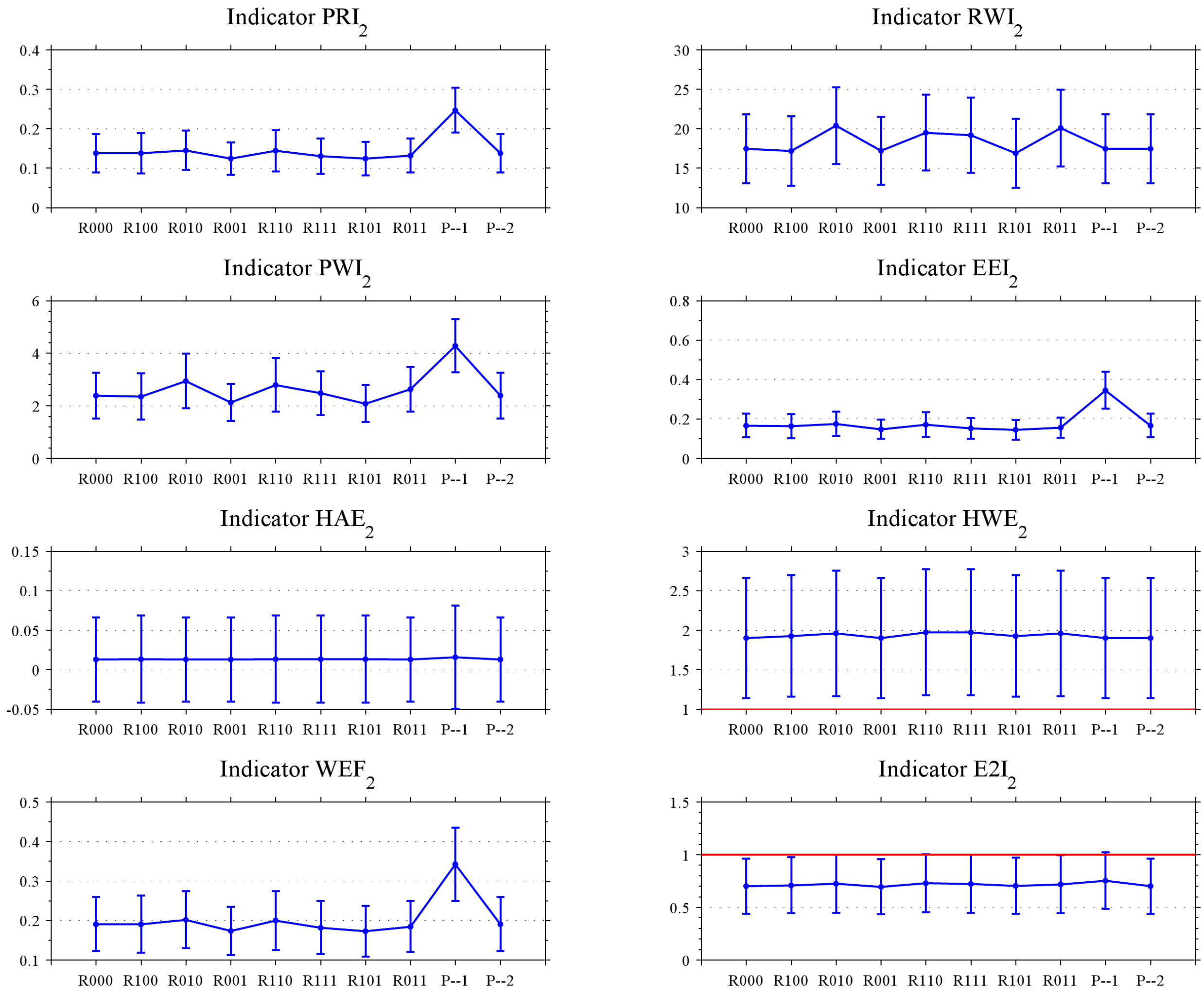

Figure 5.7: Performance of indicators for nitrogen, including the two additional scenarios P–1 and P–2.

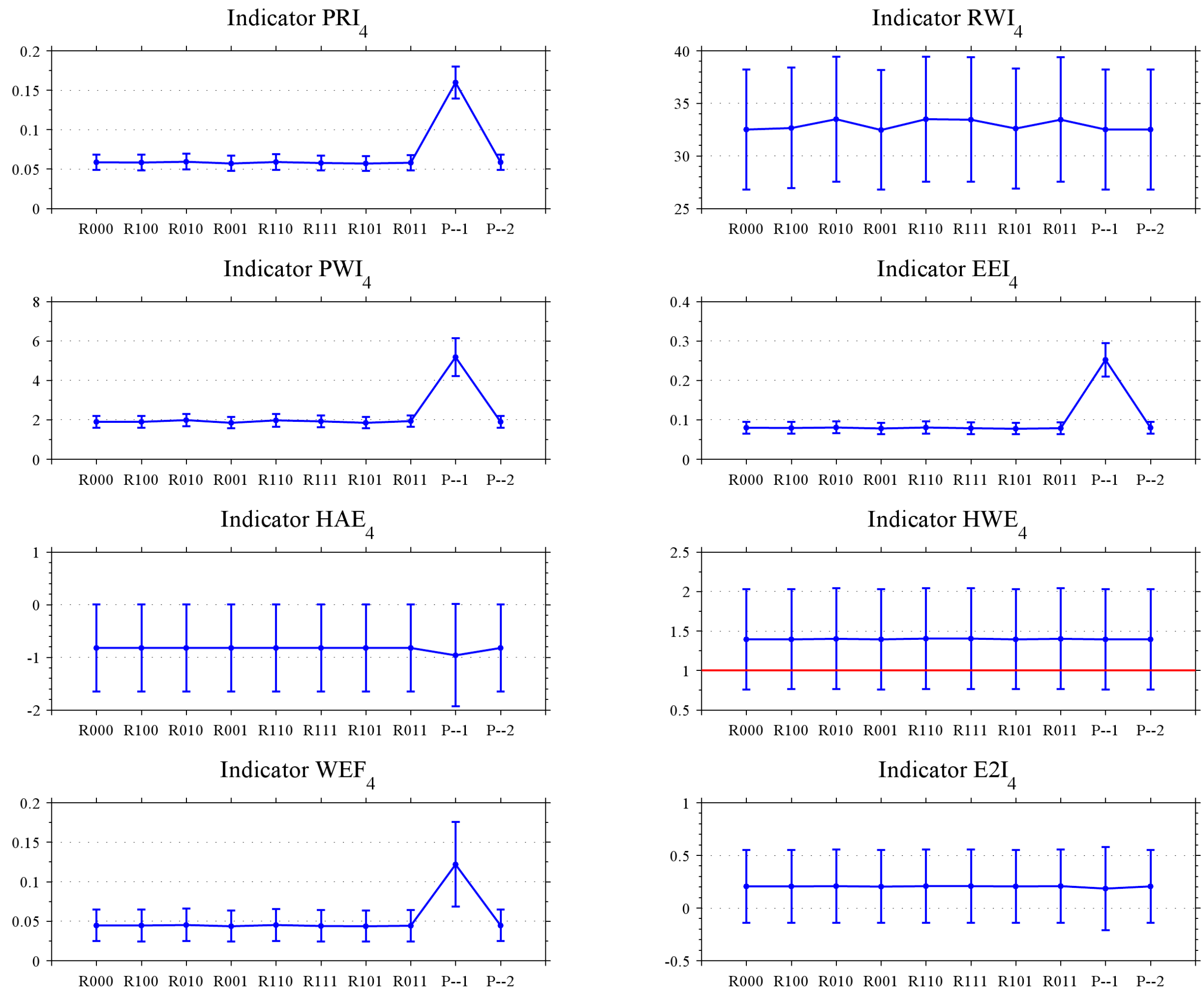

Figure 5.8: Performance of indicators for carbon, including the two additional scenarios P–1 and P–2.

decision. The effect on RWI is similar to the one experienced for the PLP scenario, in which wastes are kept constant but the need for resources is reduced (export electricity in the P–2 case).

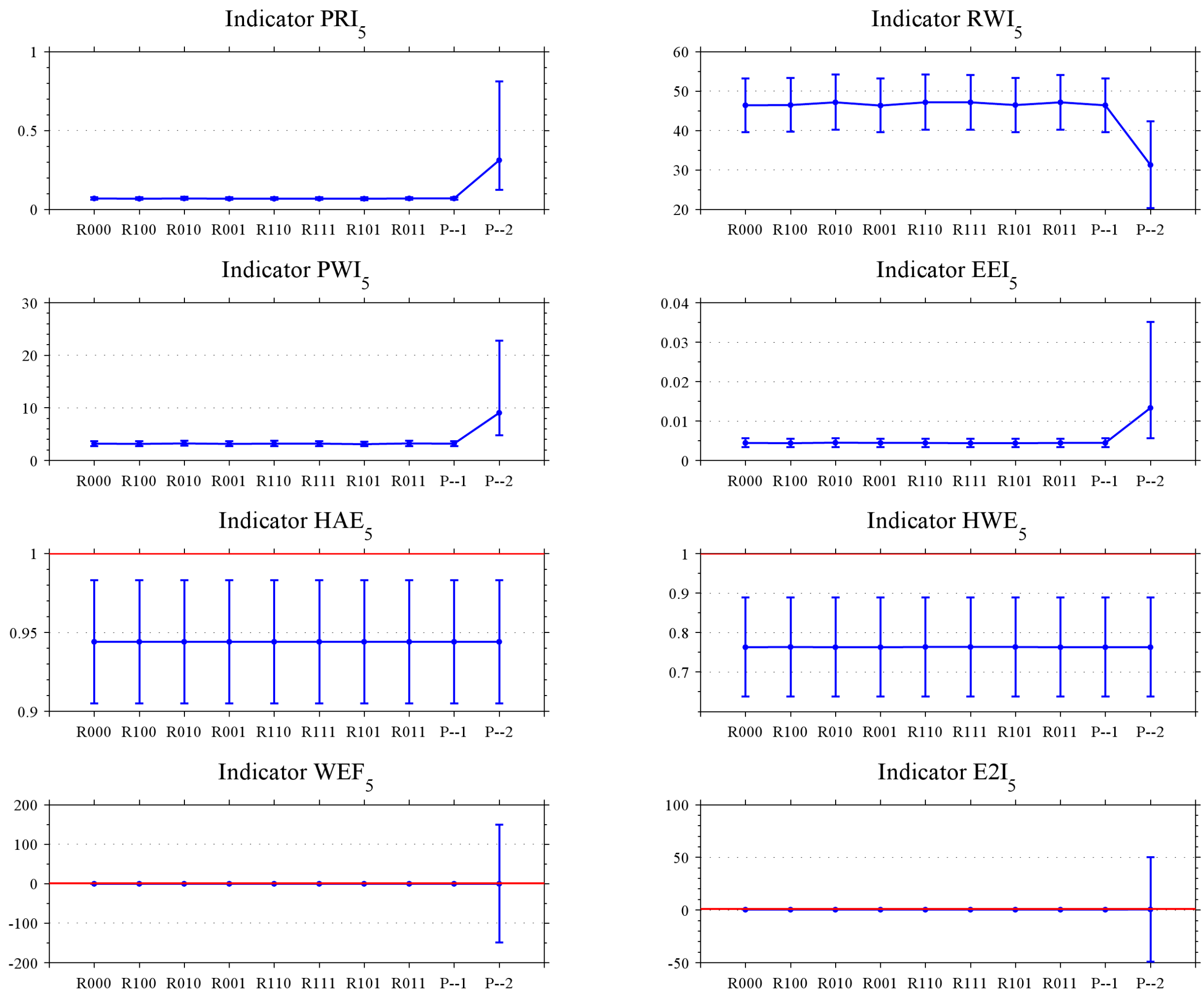

Figure 5.9: Performance of indicators for energy, including the two additional scenarios P–1 and P–2.

5.3.6 Summary of Results

When compared to the reference state (the undisturbed forest in Georgia, US), the water system tends to exhibit a higher evaporation rate, possibly due to evaporation from impervious surfaces. Releases of water via runoff are also higher than the reference state, most of the time to the detriment of soil infiltration.

In the case of N and P, the improvement of indicators seems to be related to keeping nutrients away from landfilling, either by recovering these nutrients in an early stage (UST) or as an end-of-pipe solution (MSP). Because part of the nitrogen that reaches the WWTP is lost during biological wastewater treatment, the technological solution of MSP is more effective for phosphorus, while UST is more effective for nitrogen.

On account of the structure of the indicators, together with the classification of poultry litter as a *product*, the implementation of PLP shows a poorer score relative to the other two technologies. The system (UCW) generates much less amount of products compared to the amount of resources consumed (described by PRI), so the indicators' score is more sensitive to any variation in the flow of *products*, particularly on those whose calculation involves P_k. Until now, RWI has been interpreted as the inverse of the amount of wastes generated per unit of resources consumed, thus a larger value is desirable. However, if the value of waste is kept constant, as is the case for the scenario of PLP only, R001, RWI decreases as a result of reducing the need for external resources. In principle, this could be an acceptable trade-off, but the premise under which the indicator was formulated is oriented to reduce the flow of *wastes*, thus a reduction of resources only will not report an improvement. Inversely, if all municipal solid waste is incinerated, RWI tends towards infinite, but that does not mean that the system has improved its metabolism of resources. Therefore, it is critical to analyze all indicators together to generate correct conclusions, and this is applicable to the second group of four indicators as well. Owing to the fact that indicators related with eco-effectiveness concepts are able to result in positive or negative values, specifically because emission fluxes can be entering or exiting the system, indicators HAE, HWE, WEF, and E2I must be analyzed jointly to prevent erroneous conclusions from the aggregated indicator E2I.

Revisiting the PLP case once more, if the score of indicators PRI and RWI are diminished, this means that part of the material that enters the system as animal feed (a *resource*), converted first into manure and then processed by pyrolysis, is lost via emissions or accumulated in the system. In this case, indicator EEI is suitable to providing information about the losses of a resource via emissions.

The next chapter is the last of the three case studies included in this dissertation. The sustainability measures (indicators) put in practice in the present chapter are used to define a set of targets or goals for sustainability. The RSA procedure is implemented as the tool for segregating *key* from *redundant* parameters, for the achievement of those goals.

Chapter 6

CASE STUDY PART III: Reachability of Targets

"To live is to choose. But to choose well, you must know who you are and what you stand for, where you want to go and why you want to get there." Kofi Annan

After reviewing the Upper Chattahoochee Watershed (UCW) elements in Chapter 4, and exploring the effects of different technological solutions on the environmental performance of the system (Chapter 5), this dissertation embarks on examining the possibilities for improvement by using an inverse approach. This means that instead of changing the structure of the system — by implementing a technology solution — to later assess the improvement or worsening of the indicators, a degree of improvement is defined as a goal, and through the use of Regionalized Sensitivity Analysis (RSA) the parameter space is tested with the hope of identifying the *key* parameters to attain those goals, if possible. Additionally, this third part of the UCW case study explores the uses of the Multi-sectoral Analysis (MSA) together with RSA as a framework that allows the practitioner to establish areas of interest for future research.

6.1 Specifying Sustainability Targets

For the purposes of this case study, targets are estimated assuming a nominal improvement, a percentage, from the values obtained in the *base case* scenario. Table 6.1 shows the indicators selected for this exercise and the mean value of each as obtained from the *base case*. The same table shows the calculated improved values (targets) of the indicators considering an improvement level of 30%. The calculation of the target values for indicators takes into account their mathematical behavior and the objective set for them. Their objective values are described in Table 3.2, but in general terms these can be expressed as *maximization* for the first group of indicators (PRI, RWI, PWI, and EEI) and *unity* for the the second group of indicators (HAE, HWE, WEF, and E2I). These two groups can be differentiated since the first represents efficiency concepts, while the second is built on eco-effective principles. The mathematical behavior of indicators was initially discussed throughout the analysis in Chapter 5, indicating that the responses of efficiency indicators with respect to changes in flows is easier to interpret than that of the eco-effectiveness indicators. There are some aggregated flows, in particular those associated with atmospheric emissions and processes, E_k^0 (healthy emission of the reference state) and E_k (actual emission), that have the ability of changing in direction, that is to switch from an inlet flow to an outlet flow and vice versa. This phenomenon is responsible for the mathematical behavior described in Appendix E, making their interpretation and manipulation a little more complex. Therefore, the calculation of the improved values of the indicators, shown in Table 6.1, accounts for their behavior and ensures compliance with the specified nominal improvement towards the particular objective of the indicator. In the case of the eco-effectiveness indicators, emphasis is made on reducing the distance from the *base case* value to unity, rather than increasing or reducing the actual magnitude of the indicator by a factor.

Equation (6.1) presents the set of conditional equations applicable for the indicators related with efficiency, i.e. PRI, RWI, PWI, and EEI. The improved values of indicators are estimated based on a factor that multiplies the indicator value of the *base case*.

$$\mathrm{I}_k^{imp} = \begin{cases} \mathrm{I}_k \cdot (1 + I_f) & \text{if } \mathrm{I}_k > 0 \\ \mathrm{I}_k \cdot (1 - I_f) & \text{otherwise} \end{cases} \tag{6.1}$$

where I_k is the *base case* value for a generic indicator of the kth species; I_k^{imp} is the improved value of the generic indicator; I_f is the improvement factor as a fraction 0–1. For those indicators whose the objective is unity, the improvement factor is used as the proportional reduction of the vertical distance from the *base case* scenario to unity, as shown in Equation (6.2). An exception is made for those values in the negative domain of the indicator (see Appendix E) in which case I_k^{imp} is calculated using the improvement factor as a simple multiplier,

$$\mathrm{I}_k^{imp} = \begin{cases} \mathrm{I}_k - (\mathrm{I}_k - 1) \cdot I_f & \text{if } \mathrm{I}_k > 1 \\ \mathrm{I}_k + (\mathrm{I}_k - 1) \cdot I_f & \text{if } 0 < \mathrm{I}_k < 1 \\ \mathrm{I}_k \cdot (1 + I_f) & \text{otherwise} \end{cases} \tag{6.2}$$

The improved value of E2I is calculated in Equation (6.3) as the sum of the improvements of HAE, HWE, and WEF, thus, the factor I_f is being considered in an indirect way. This approach is preferred to prevent the model from moving towards misleading values of E2I, i.e., an E2I value tending to unity without checking that the other three indicators (HAE, HWE, and WEF) are actually improving.

$$\mathrm{E2I}_k^{imp} = \beta_{1,k}\left(\mathrm{HAE}_k^{imp}\right) + \beta_{2,k}\left(\mathrm{HWE}_k^{imp}\right) + \beta_{3,k}\left(\mathrm{WEF}_k^{imp}\right) \tag{6.3}$$

As shown in Table 6.1, this analysis is not carried out for all the possible indicators per species but for a total of eleven, with at least one indicator per species. The indicators selection is based on possible interests from the view point of regulation, such as water efficiency PRI_1, energy efficiency PRI_5, aquatic emissions of nitrogen HWE_1 and phosphorus HWE_3 (typically associated with eutrophication), air emissions of carbon HAE_4 (mostly related with global warming), and eco-efficiency and eco-effectiveness, EEI and E2I respectively, of nitrogen, phosphorus and carbon. Because the purpose of the case study is to illustrate the capacity of the MSA model for identifying key parameters, any level of improvement could have been selected. Nonetheless, a 30% is considered with the particular interest of moving the improved values far enough from the *base case*, but yet at a reachable level for most indicators, to make the results more attractive.

Table 6.1: Indicators selected for Regionalized Sensitivity Analysis (RSA) and the values used to define the improvement goals, using $I_f = 0.30$.

Indicator	***Base case* values**[a]	**Improved value**[a]
PRI_1	1.05	1.36
EEI_2	0.17	0.22
HWE_2	1.90	1.63
$E2I_2$	0.70	0.79
EEI_3	1.48	1.92
HWE_3	0.75	0.82
$E2I_3$	0.66	0.76
EEI_4	0.08	0.10
HAE_4	(0.82)	(1.07)
$E2I_4$	0.21	0.18
PRI_5	0.07	0.09

[a] Values in parenthesis are negative.

6.2 Identifying Key Processes for Sustainability

Regionalized Sensitivity Analysis (RSA), explained in Section 2.4, is the procedure used for the identification of those parameters that are key to reaching the targets specified in Table 6.1. By revealing the key parameters it is also possible to determine which sectors and processes are *critical*. In general terms, the segregation of *critical* from *redundant* parameters is comprised of three steps:

(i) classifying the model results, and the corresponding parameter vector, into behaviors B and non-behaviors NB. This depends on whether the improved value of the indicator under analysis is met or exceeded (B) or not (NB). The procedure is repeated for every single indicator that is investigated, so that in this study case RSA is activated for a total of eleven times to include all indicators mentioned in Table 6.1.

(ii) performing the Kolmogorov-Smirnov (K-S) two-sample test (two-sided version) for each parameter based on the information generated in the previous step.

(iii) Based on the significance level reported by the K-S test, and for the purposes of this case study, classifying parameters either as *critical* or *redundant*.

To illustrate in a visual manner the results of these three steps, Figure 6.1 is generated for parameter α_{142}, 'phosphorus leaching factor'. From the analysis indicator HWE_2, Figure 6.1(a) shows that there is no difference between the cumulative density functions of the behavior and the non-behavior, therefore the parameter is not *critical* for the indicator of healthy aquatic emissions of nitrogen. However, when examining the indicator of healthy aquatic emissions for phosphorus (HWE_3), the parameter does exhibit a statistically significant difference between behavior and non-behavior as shown in Figure 6.1(b).

6.3 Results and Discussion

In the task of improving the indicators in Table 6.1 by 30%, a total of 105 parameters, out of 574, were found to be *critical* for at least one indicator. No key parameters were found for indicators PRI_1 and PRI_5 for different reasons. PRI_1 is already larger than unity, meaning that more water is returned to surface and ground water sources compared to

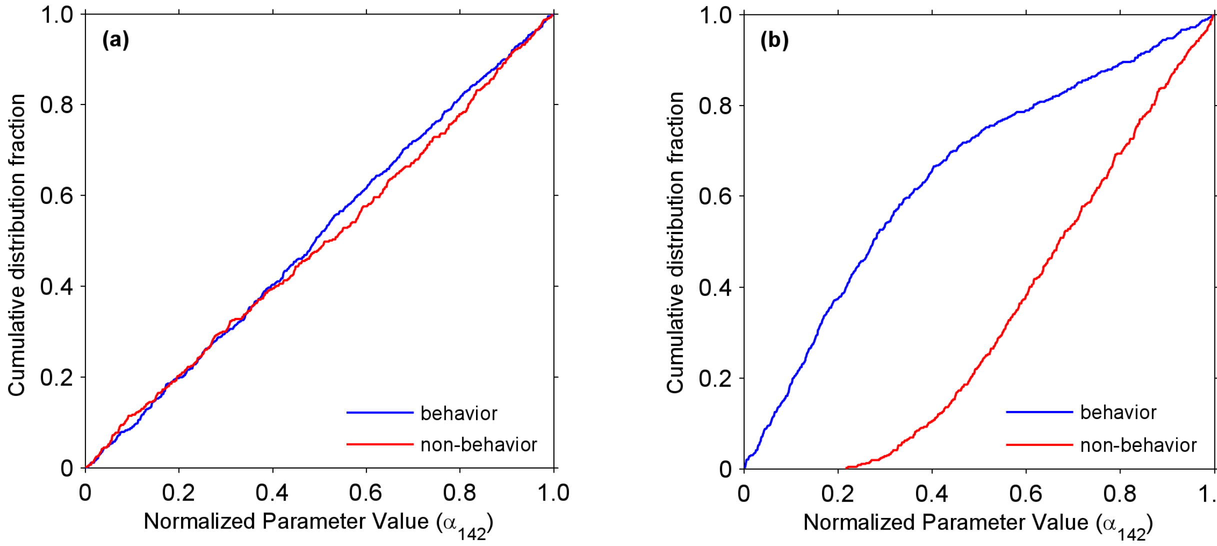

Figure 6.1: Segregation of cumulative density function curves corresponding to the behavior and non-behavior of parameter α_{142}, 'phosphorus leaching factor'. (a) shows the result associated with indicator HWE_2 (not significantly different), and (b) presents curves related to HWE_3 (significantly different).

water withdrawals (see Section 5.3.1 for a more detailed explanation). Thus, due to the characteristics of the water cycle, and not the system performance, it is improbable that a 30% level of improvement will take place for indicator PRI_1. On the other hand, the current system's structure, and the range assumed for the parameters associated with the energy sector, e.g., *efficiency of coal combustion*, does not allow indicator PRI_5 to meet the 30% improvement. Therefore, the following analysis is devoted to the remaining nine indicators.

The number of critical parameters per indicator varies from 13 to 31, as shown in Table 6.2, but there is a clear divide of two groups, those under 17 and those above 26. The complexity of the indicator, conceived as the degree of connection to processes and flows, is reflected in the number of critical parameters, thus, most composite indicators, i.e. EEI and E2I, have more than 26. However, this is not true for indicator $E2I_2$ and EEI_4, possibly because for the UCW case these indicators are not associated with a high number of critical parameters. EEI_4 is highly dependent on carbon emissions; therefore consistent with the lower complexity of HAE_4. On the other hand, the fact that $E2I_2$ and HWE_2 are related to fewer critical parameters suggests that the improvement of HAE_2 (not analyzed in this case study) might also depend on a reduced number of parameters.

Table 6.2: Number of critical parameters per indicator.

Eco-efficiency, nitrogen	EEI_2	28
Healthy aquatic emission, nitrogen	HWE_2	13
Eco-effectiveness, nitrogen	$E2I_2$	16
Eco-efficiency, phosphorus	EEI_3	31
Healthy aquatic emission, phosphorus	HWE_3	17
Eco-effectiveness, phosphorus	$E2I_3$	30
Eco-efficiency, carbon	EEI_4	16
Healthy atmospheric emission, carbon	HAE_4	16
Eco-effectiveness, carbon	$E2I_4$	26

Figure 6.2 expands the analysis even further by reporting the number of *critical* parameters per industrial sector, Figure 6.2(a), and classified by the number of indicators that they affect, Figure 6.2(b). It can be observed that the food sector is related to the largest number of *critical* parameters, followed by the water, forestry, and energy sectors, while the sector of waste management is associated with the least number of *critical* parameters. This means that management strategies of the food sector, which includes the poultry industry in the specific case of the UCW, has a strong effect on the performance of the indicators towards the sustainability targets. Focusing now on Figure 6.2(b), it is evident that most of the parameters, about 55%, have a critical influence on only one indicator while only five of the parameters, listed in Table 6.3, are key to five indicators each. Interestingly, four of these parameters are related to climatic conditions and have a significant effect on surface runoff, and consequently the aquatic emissions of N, P, and C. Therefore, surface runoff management appears to be critical to achieve a 30% improvement in the eco-effectiveness

of the system. The fifth parameter, α_{143}, has a direct influence on the amount of organic fertilizer (manure or treated municipal sludge) that is applied to the soil. Because using an organic source of nutrient does not necessarily match the exact ratio of nutrients required by the plant, it could happen that one or more nutrients will be in excess. For instance, if nitrogen is the reference nutrient for calculating the amount of poultry litter to be applied, given the characteristics of this fertilizer, it is possible that phosphorus would be in excess; therefore affecting processes associated with N and P at the same time.

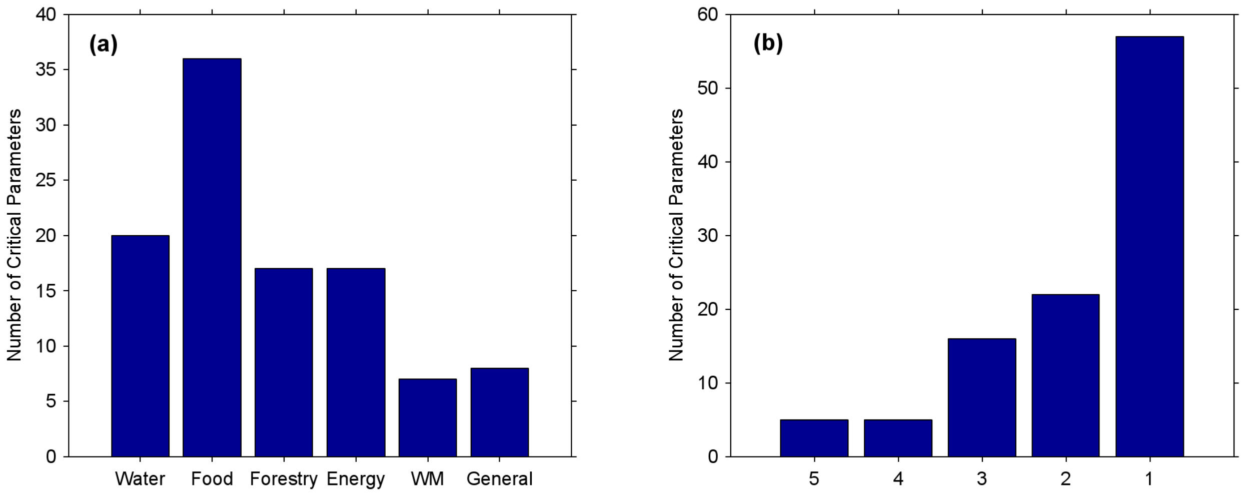

Figure 6.2: Analysis of number of critical parameters. (a) represents the number of critical parameters per industrial sector: water, food, forestry, energy, waste management (WM), and general (refers to those parameters that are related to two or more sectors, e.g. *Plant Available Nitrogen*). (b) shows the number of critical parameters for each frequency classification, i.e. from five indicators to one indicator. In other words, the number of parameters that are critical for a number of indicators at the same time.

A more detailed analysis can be carried out by investigating those specific *critical* parameters associated with each indicator. Table 6.4 lists the *critical* parameters for indicator EEI_2 with no specific order excepting that indicators are grouped by sector. Nine of the twenty-eight parameters are related to the poultry industry, suggesting that attention must be paid to related flows in order to improve the eco-efficiency of the system with respect to nitrogen. Solutions such as reducing excess N in poultry fodder or better management of poultry litter to minimize ammonia volatilization might be appropriate. Although Urine

Table 6.3: Critical parameters associated with the improvement of five indicators.

Parameter		**Units**	**Indicators associated with**
Pervious area infiltration index	α_{59}	ratio	HWE_2, $E2I_2$, HWE_3, $E2I_3$, $E2I_4$
Average monthly cloudiness	α_{61}	%	HWE_2, $E2I_2$, HWE_3, $E2I_3$, $E2I_4$
Average air temperature	α_{534}	°C	HWE_2, $E2I_2$, HWE_3, $E2I_3$, $E2I_4$
Average latitude of the system	α_{536}	degrees	HWE_2, $E2I_2$, HWE_3, $E2I_3$, $E2I_4$
Plant Available Nitrogen (PAN)	α_{143}	ratio	EEI_2, HWE_2, $E2I_2$, EEI_3, $E2I_3$

Separation Technology (UST) decreases N emissions to air from wastewater treatment plants (WWTP), it seems that manipulating the parameter associated with the denitrification rate of the biological wastewater treatment, α_{106}, has a more significant effect on reducing these emissions given that not all the nitrogen sent to WWTPs is from urine, but also from other sources, e.g., industrial.

Strategies for reducing N loads in urban surface runoff (α_{231}) are *critical* for a better performance of the system by reducing aquatic emissions, and consequently, the improvement of the eco-efficiency indicator EEI_2.

In the energy sector, the reduction in natural gas use appears to be *critical* for EEI_2. Pyrolysis of sludge (α_{195}) and the amount of CCP (coal combustion products) sent for landfilling (α_{197}) have a direct influence on aquatic emissions through leaching, hence their relevance to meeting the target, the first possibly by increasing and the second by decreasing its magnitude. The CCP not sent to landfill is considered a product, which improves EEI_2 as well. On the other hand, the analysis presented in Section 5.3.2 showed that introducing pyrolysis of poultry litter has a negative effect on the performance of most indicators, and for this reason the relevance of α_{193} for improvement lies most probably in being as small as possible.

Table 6.4: Critical parameters for indicator EEI_2, eco-efficiency of nitrogen.

Parameter identification code and description[b]		Units	Sector[a]
α_{60}	No. of days with >.01 of precipitation	events per y	1
α_{231}	Surface runoff nutrients (impervious areas)	N content	1
α_{504}	Total population	cap $\times 10^3$	1
α_{106}	WWTP — plant-wide N_2 release rate	ratio	1
α_{162}	Poultry manure production rate (per kg of B_w)	$\mathrm{kg\,kg^{-1}\,y^{-1}}$	2
α_{315}	Fertilization rate: crop and pasture	$\mathrm{kg\,N\,ha^{-1}\,y^{-1}}$	2
α_{132}	Crop and pasture area fertilized	percent	2
α_{510}	Inventory of poultry	heads $\times 10^3$	2
α_{543}	Average poultry weight	$\mathrm{kg\,head^{-1}}$	2
α_{135}	Nitrogen volatilization from poultry litter	ratio	2
α_{328}	Nutrient content of fresh poultry litter	N content	2
α_{332}	Nutrient content of fresh poultry litter	Water content	2
α_{203}	Poultry annual breed factor	ratio	2
α_{327}	Water content per fresh kg of cattle manure	Water content	2
α_{357}	Yard/agricultural residue	Water content	2
α_{407}	Live animal — poultry	N content	2
α_{542}	Average cattle weight	$\mathrm{kg\,head^{-1}}$	2
α_{547}	Milk yield per cow	$\mathrm{kg\,head^{-1}\,y^{-1}}$	2
α_{128}	Denitrification rate in forested areas	$\mathrm{kg\,P\,ha^{-1}\,y^{-1}}$	3
α_{208}	DO and IN natural gas combustion efficiency	ratio	3
α_{362}	Paper and paperboard	Water content	3
α_{444}	Natural gas composition — dry basis	N content	4
α_{518}	capacity for power generation - coal	MW	4
α_{181}	Industrial energy supplied by natural gas	ratio	4
α_{195}	Treated sludge sent to pyrolysis	ratio	5
α_{197}	CCP sent to landfill	ratio	5
α_{193}	Poultry manure sent to pyrolysis	ratio	5
α_{143}	Plant Available Nitrogen (PAN)	ratio	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] DO domestic use; IN industrial use; CCP coal combustion products; B_w body mass; WWTP wastewater treatment plant.

Indicator HWE_2, Table 6.5, is highly influenced by climatic conditions related to surface runoff such as precipitation and other parameters that control evaporation (and the availability of water for runoff). Additionally, reducing the parameters that control the nitrogen content in leachate from forests (α_{212}) and grassland (α_{212}) have a beneficial effect on the health of nitrogen aquatic emissions. The seemingly peculiar participation of nitrogen and energy content in fruits might have to do with the leaching associated with food sent for landfilling and composting. However, this leaves the unanswered question of why other types of food are not relevant, notably because other foods such as cereal and meat have a larger amount of nitrogen. The parameter for nutrient content in the O horizon of undisturbed forests (α_{476}) is significant since it defines the reference state against which actual aquatic emissions are compared to when calculating indicator HWE_2. However, this significance is less functional in the sense that management strategies and structural changes of the system cannot change the reference state, but is informative with respect to the importance of how the reference state is described.

Table 6.5: Critical parameters for indicator HWE_2, healthy aquatic emission of nitrogen.

Parameter identification code and description		**Units**	**Sector**[a]
α_{59}	Pervious area infiltration index	ratio	1
α_{61}	Average monthly cloudiness	percentage	1
α_{534}	Average air temperature	°C	1
α_{536}	Average latitude of the system	degrees	1
α_{557}	Precipitation	mm	1
α_{231}	Surface runoff nutrients (impervious areas)	N content	1
α_{212}	Grassland floor nutrient content[b]	ratio	2
α_{363}	Fruit	N content	2
α_{366}	Fruit	Energy content	2
α_{213}	Forestland floor nutrient content[b]	ratio	3
α_{143}	Plant Available Nitrogen (PAN)	ratio	23
α_{141}	Nitrogen leaching factor	ratio	23
α_{476}	O horizon layer in undisturbed forests	N content	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] With respect to an undisturbed forest.

Knowing that indicator $E2I_2$ is a function of HWE_2 explains why most of the runoff-associated parameters in Table 6.5 are also present in Table 6.6, but this time with the addition of one parameter associated with the atmospheric exchange of nitrogen, nitrogen fixation rate in forested areas (α_{125}). In Section 4.2.2, it was found that the largest atmospheric flows are those related to fuel combustion for purposes other than power generation, exceeding by 10-fold the amount of nitrogen fixated, suggesting that α_{125} is relevant because it is part of the calculation of E_2^0, the emission of the reference state (undisturbed forest).

The emissions from natural gas combustion (α_{444}), and coal combustion (α_{452} and α_{455}) are *critical* to improve the N air emission component of the eco-effectiveness performance. Sending CCP to landfill (α_{197}) can have a negative effect on the amount of N leached (part of HWE_2), while accumulating N in the form of landfilled CCP worsens WEF_2, both key for the performance of $E2I_2$.

Table 6.6: Critical parameters for indicator $E2I_2$, eco-effectiveness of nitrogen.

Parameter identification code and description		**Units**	**Sector**[a]
α_{59}	Pervious area infiltration index	ratio	1
α_{61}	Average monthly cloudiness	percentage	1
α_{534}	Average air temperature	°C	1
α_{536}	Average latitude of the system	degrees	1
α_{557}	Precipitation	mm	1
α_{231}	Surface runoff nutrients (impervious areas)	N content	1
α_{57}	Effective impervious areas	ratio	1
α_{213}	Forestland floor nutrient content[b]	ratio	3
α_{125}	Nitrogen fixation rate — forested areas	$\mathrm{kg\,N\,ha^{-1}\,y^{-1}}$	3
α_{455}	Coal composition — dry basis	Energy content	4
α_{444}	Natural gas composition - dry basis	N content	4
α_{452}	Coal composition — dry basis	N content	4
α_{197}	CCP[c] sent to landfill	ratio	5
α_{143}	Plant Available Nitrogen (PAN)	ratio	23
α_{141}	Nitrogen leaching factor	ratio	23
α_{476}	O horizon layer in undisturbed forests	N content	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] With respect to an undisturbed forest.
[c] CCP coal combustion product.

Similar to EEI_2, the equivalent indicator for phosphorus (EEI_3) is also greatly influenced by the poultry industry, but this time, because there is no atmospheric component, the emphasis is on poultry litter as a product. The only interaction with atmospheric processes is the P emission from coal combustion, so it is logical to have α_{453} as a *critical* parameter, see Table 6.7. The forestry industry makes its first representative appearance by including paper and sawmill material. The latter (α_{77}) can be seen as a description of how much P, in the form of semi-processed wood, is sent outside the system as a product. The amount of phosphorus sent to landfill or as a product to other systems is also *critical*, as revealed by the participation of parameters that define the amount of paper and CCP that is either landfilled (leaching) or sent to other systems categorized as a *product* flow: 'CCP sent to landfill' (α_{197}), 'MSW paper disposal', (α_{85}), and 'paper/paperboard recovery' factor for recycling (α_{89}). The concentration of P associated with these materials, paper and paperboard (α_{362}), and coal (α_{453}) is also relevant. Therefore, strategies for increasing the recycling of paper waste and the use of CCPs are important.

When referring specifically to the eco-efficiency of the system in terms of P, finding the parameter for the P content in municipal wastewater (α_{216}) *critical*, and not the parameter of UST (urine separation technology) implementation, suggests that the contribution of P in municipal wastewater from sources other than urine seems to be relevant. Moreover, the model appears to be more sensitive to the improvement achieved by reducing the content of P in human urine, α_{220}, which will reduce the amount of P loss through septic tanks, than recovering P using UST.

The improvement of indicator HWE_3, as usual for aquatic emissions, is associated with runoff and other climatic processes that affect runoff, see Table 6.8. Similar to HWE_2, urban runoff is more significant than the contribution from pervious areas (not part of the *critical* parameters). Leaching of P from pervious areas, particularly in forested areas, is indeed relevant as suggested by the presence of parameters that describe the area of forests that is fertilized (α_{131}) and the rate at which the P present is leached (α_{142}). The P load in sewage (α_{216}) and the amount of P recovered using sludge pyrolysis (α_{195}) are both *critical* as they prevent P from leaching after treated sludge is sent to landfills. The possible connection

Table 6.7: Critical parameters for indicator EEI_3, eco-efficiency of phosphorus.

Parameter identification code and description[b]		Units	Sector[a]
α_{216}	Untreated municipal wastewater	P content	1
α_{557}	Precipitation	mm	1
α_{232}	Surface runoff nutrients (impervious areas)	P content	1
α_{217}	Untreated municipal wastewater	BOD content	1
α_{220}	Human urine	P content	1
α_{162}	Poultry manure production rate (per kg of B_w)	$\mathrm{kg\,kg^{-1}\,y^{-1}}$	2
α_{315}	Fertilization rates: crop and pasture	N content	2
α_{132}	Crop and pasture area fertilized	percent	2
α_{510}	Inventory of poultry	heads $\times 10^3$	2
α_{543}	Average poultry weight	$\mathrm{kg\,head^{-1}}$	2
α_{328}	Nutrient content of fresh poultry litter	N content	2
α_{332}	Water content of fresh poultry litter	Water content	2
α_{124}	Nitrogen fixation rate — grassland	$\mathrm{kg\,N\,ha^{-1}\,y^{-1}}$	2
α_{159}	Poultry selling rate	head/head	2
α_{202}	Cattle annual breed factor	head/head	2
α_{308}	Fertilization rates: grass and lawn	P content	2
α_{329}	Nutrient content of fresh poultry litter	P content	2
α_{334}	Nutrient content per fresh kg of swine manure	P content	2
α_{408}	Live animal — poultry	P content	2
α_{423}	Poultry feed requirements	P content	2
α_{546}	Fraction of layers	ratio	2
α_{77}	Sawmill efficiency	ratio	3
α_{89}	Paper/paperboard recovery factor	ratio	3
α_{67}	Hardwood — live trees average net growth	$\mathrm{m^3\,ha^{-1}\,y^{-1}}$	3
α_{453}	Coal composition - dry basis	P content	4
α_{195}	Treated sludge sent to pyrolysis	ratio	5
α_{197}	CCP sent to landfill	ratio	5
α_{193}	Poultry manure sent to pyrolysis	ratio	5
α_{85}	MSW paper disposal factor	ratio	5
α_{143}	Plant Available Nitrogen (PAN)	ratio	23
α_{142}	Phosphorus leaching factor	ratio	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] BOD Biochemical oxygen demand; CCP coal combustion products; B_w body mass.

among aquatic emissions, coal P content (α_{453}), and coal combustion efficiency (α_{167}) is the production of CCPs that is partly sent to landfills and contributes to P leachate.

Table 6.8: Critical parameters for indicator HWE_3, healthy aquatic emissions of P.

Parameter identification code and description[b]		**Units**	**Sector**[a]
α_{59}	Pervious area infiltration index	ratio	1
α_{61}	Average monthly cloudiness	percentage	1
α_{534}	Average air temperature	°C	1
α_{536}	Average latitude of the system	degrees	1
α_{216}	Untreated municipal wastewater	P content	1
α_{60}	No. of days with >.01 inches of precipitation	events per year	1
α_{232}	Surface runoff nutrients (impervious areas)	P content	1
α_{105}	WWTP — plant-wide BOD removal rate	ratio	1
α_{429}	Pig feed requirements	Energy content	2
α_{160}	Hogs and pigs selling rate	ratio	2
α_{131}	Forest area fertilized	percent	3
α_{69}	Hardwood — live trees average annual removal	$m^3\,ha^{-1}\,y^{-1}$	3
α_{453}	Coal composition — dry basis	P content	4
α_{167}	Coal power plant energy efficiency	ratio	4
α_{195}	Treated sludge sent to pyrolysis	ratio	5
α_{142}	Phosphorus leaching factor	ratio	23
α_{477}	O horizon layer in undisturbed forests	P content	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] WWTP wastewater treatment plant; BOD Biochemical oxygen demand.

The eco-effectiveness indicator in terms of P, i.e. $E2I_3$, is sensitive to surface runoff from impervious areas as indicated by the high level of significance of the phosphorus concentration in runoff (α_{232}), see Table 6.9. Leaching from pervious areas, particularly crop and pasture areas, is *critical* for the aquatic emissions component of the eco-effectiveness indicator because of the presence of parameters that control the area to be fertilized (α_{132}) and the rate at which nutrient is supplemented (α_{315}). If an organic nutrient source is used as fertilizer (e.g. manure or sludge), the case study calculates the nutrient application in N terms. Therefore, the parameters α_{315}, which is the recommended application rate of N for crops and pastures, and α_{143}, the plant available nitrogen parameter, become relevant for the amount of P applied to the soil that contributes to leaching. Background leaching (no fertilization) from forestland, controlled by the nutrient content of the forest floor (α_{213}), is found to be relevant.

Because of the limited participation of phosphorus in atmospheric processes, wet (α_{497}) and dry deposition (α_{501}) play a significant role on $E2I_3$ via their influence on HAE_3. It happens similarly with the P content in coal (α_{453}), which is the basis for estimating the emission of P particles during coal combustion. Of these three parameters, only the emission of P from coal combustion can be controlled locally.

For indicator $E2I_3$, all three technologies, urine separation technology (UST), municipal sludge pyrolysis (MSP), and poultry litter pyrolysis (PLP), are key in achieving the 30% improvement target. This result can be complemented with the analysis performed in Chapter 5 to understand in which way these technologies are *critical*. Chapter 5 revealed that UST and MSP have a positive effect on the performance of indicators, while PLP has a negative effect, suggest that the improvement of $E2I_3$ is most likely achieved if UST or MSP implementation is maximized, α_{98} and α_{195} respectively, while PLP is minimized (α_{193}). The collection efficiency of the urine separation technology, α_{97}, is also identified as key, implying that enhancing the efficiency of the urine separation device can contribute positively to reaching the proposed target.

The critical parameters for indicator EEI_4, in Table 6.10, have a strong connection to the energy sector. Because the eco-efficiency indicator is a function of the *product* flow of the system and, air and aquatic emissions generated within the system, the importance of energy-related parameters are due to their relevance for the air emissions derived from fuel consumption. The content of carbon in coal (α_{455}) and gasoline (α_{462}) are *critical*, but difficult to manage; however, reducing transportation (α_{184}) and industrial energy use (α_{180}) are more achievable tasks. The fact that composition of fuels is part of the *critical* parameters, particularly the energy content of coal (α_{455}) and gasoline (α_{463}), says something about the

Table 6.9: Critical parameters for indicator $E2I_3$, eco-effectiveness of phosphorus.

Parameter identification code and description		Units	Sector[a]
α_{59}	Pervious area infiltration index	ratio	1
α_{61}	Average monthly cloudiness	percentage	1
α_{534}	Average air temperature	°C	1
α_{536}	Average latitude of the system	degrees	1
α_{216}	Untreated municipal wastewater	P content	1
α_{232}	Surface runoff nutrients (impervious areas)	P content	1
α_{497}	Nutrient content in wet deposition	P content	1
α_{97}	Efficiency of urine separation device	ratio	1
α_{98}	Urine separation implementation ratio	ratio	1
α_{162}	Poultry manure production rate (per kg of B_w)	$\mathrm{kg\,kg^{-1}\,y^{-1}}$	2
α_{315}	Fertilization rate: crop and pasture	N content	2
α_{132}	Crop and pasture area fertilized	percent	2
α_{510}	Inventory of poultry	heads $\times 10^3$	2
α_{543}	Average poultry weight	$\mathrm{kg\,head^{-1}}$	2
α_{158}	Cattle selling rate (a ratio of inventory)	head/head	2
α_{200}	Vegetables crop yield factor	$\mathrm{cwt\,acre^{-1}}$	2
α_{370}	Cereal	Energy content	2
α_{390}	All hay (including alfalfa)	Energy content	2
α_{213}	Forestland floor nutrient content[b]	ratio	3
α_{453}	Coal composition - dry basis	P content	4
α_{452}	Coal composition - dry basis	N content	4
α_{179}	Commercial energy supplied by biomass	ratio	4
α_{185}	Transportation energy supplied by natural gas	ratio	4
α_{195}	Treated sludge sent to pyrolysis	ratio	5
α_{197}	CCP[c] sent to landfill	ratio	5
α_{193}	Poultry manure sent to pyrolysis	ratio	5
α_{143}	Plant Available Nitrogen (PAN)	ratio	23
α_{142}	Phosphorus leaching factor	ratio	23
α_{477}	O horizon layer in undisturbed forests	P content	23
α_{501}	Nutrient content in dry deposition	P content	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] With respect to an undisturbed forest.
[c] CCP coal combustion products.

positive effect that the efficiency of combustion processes of coal and gasoline can have on the improvement of EEI_4. The efficiency of the internal combustion of gasoline (α_{205}) is found to be *critical* but the efficiency of coal combustion is substituted by the presence of the parameter associated with the local capacity for power generation using coal (α_{518}). The latter means that moving away from coal-fired generation brings more benefits than improving its efficiency. A similar logic can be applied to the parameter of energy content of wood materials (α_{346}), which suggests that improving the efficiency of wood combustion (used as firewood and for industrial energy) could also be influential.

Poultry manure production (α_{162}) and waste paper recovery (α_{89}) are both positively correlated with the flow of *products*, hence their relevance for EEI_4. On the other hand, the generation of municipal solid waste (parameter α_{84}) can affect EEI_4 in two ways: (i) by reducing the amount of paper sent to landfills, which has a direct effect on C leaching, or (ii) by increasing the amount of paper recycled, in conjunction with the waste paper recovery parameter (α_{89}). The latter seems to be the case for the UCW as suggested by absence of leaching parameters, e.g., from the forest floor with its high content of C, from the list of *critical* parameters (Table 6.10).

Most of the parameters that are *critical* for EEI_4, particularly those associated with air emissions from fuel combustion, are present in Table 6.11 for indicator HAE_4. However, there are three main differences between the *critical* parameters of these two indicators. First, total population (α_{504}), as a consumption driver, is now relevant. Carbon sequestration in forest biomass, above-ground (α_{121}) and below-ground (α_{123}), and soil organic matter (α_{478}) are key to reverse the typically outgoing flow of carbon from urban areas into an incoming flow, as is the case of forests (the reference state). Sawmill efficiency (α_{77}), and indirectly the carbon content of wood (α_{345}), dictates how much carbon in sawmill residue is available for

Table 6.10: Critical parameters for indicator EEI_4, eco-efficiency of carbon.

Parameter identification code and description[b]		**Units**	**Sector**[a]
α_{162}	Poultry manure production rate (per kg of B_w)	$\mathrm{kg\,kg^{-1}\,y^{-1}}$	2
α_{323}	Nutrient content per fresh kg of cattle manure	N content	2
α_{426}	Pig feed requirements	Fat content	2
α_{345}	Wood (average softwood and hardwood)	C content	3
α_{89}	Paper/paperboard recovery factor	ratio	3
α_{360}	Paper and paperboard	C content	3
α_{346}	Wood (average softwood and hardwood)	Energy content	3
α_{205}	Internal combustion efficiency for engines	ratio	4
α_{455}	Coal composition — dry basis	Energy content	4
α_{184}	Transportation energy use per capita	$\mathrm{MWh\,y^{-1}}$	4
α_{454}	Coal composition — dry basis	C content	4
α_{463}	Gasoline composition	Energy content	4
α_{518}	Capacity for power generation — coal	MW	4
α_{180}	Industrial energy use per capita	$\mathrm{MWh\,y^{-1}}$	4
α_{462}	Gasoline composition	C content	4
α_{84}	MSW disposal per capita	$\mathrm{kg\,d^{-1}}$	5

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.

[b] DO domestic use; IN industrial use; CCP coal combustion products; B_w body mass; WWTP wastewater treatment plant.

use as biomass for energy purposes (combustion); therefore, a reduced value of the parameter improves HAE_4.

Recovered food (parameter α_{90}) is sent to composting, as opposed to incineration and landfilling. Although the composting process is known by the stabilization of organic material at the cost of significant loss of nutrient to the atmosphere, the loss per kilogram of carbon (≈53%) is less than the incineration process (≈98%) but still more than the emission released from landfill operations (≈25% after a nearly 50% gas captured for energy generation). Therefore, it is not entirely clear which strategy is adequate to achieve the desired improvement, but it seems that by not reporting the parameter that divides the waste food flow to either landfill or incineration (α_{93}) as *critical*, the right choice under uncertainty is composting, at least in terms of carbon air emissions.

Table 6.11: Critical parameters for indicator HAE_4, Healthy air emissions of carbon.

Parameter identification code and description[b]		Units	Sector[a]
α_{504}	Total population	cap $\times 10^3$	1
α_{135}	Nitrogen volatilization from poultry litter	ratio	2
α_{131}	Forest area fertilized	percent	3
α_{345}	Wood	C content	3
α_{77}	Sawmill efficiency	ratio	3
α_{121}	Above-ground biomass growth (forests)	$\mathrm{t\,ha^{-1}\,y^{-1}}$	3
α_{123}	below-ground/above-ground biomass (forests)	ratio	3
α_{205}	Internal combustion efficiency for engines	ratio	4
α_{455}	Coal composition — dry basis	Energy content	4
α_{184}	Transportation energy use per capita	$\mathrm{MWh\,y^{-1}}$	4
α_{454}	Coal composition — dry basis	C content	4
α_{463}	Gasoline composition	Energy content	4
α_{90}	Food recovery factor	ratio	5
α_{141}	Nitrogen leaching factor	ratio	23
α_{478}	O horizon layer in undisturbed forests	C content	23
α_{501}	Nutrient content in dry deposition	P content	23

[a] Sectors are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] DO domestic use; IN industrial use; CCP coal combustion products; B_w body mass; WWTP wastewater treatment plant.

Similar to many of the previous indicators related directly or indirectly to aquatic emissions, the concentration of carbon in runoff from impervious areas (α_{233}) and infiltration (α_{140}) from forest (described by α_{213} and α_{131}) and grassland (related to α_{315} and α_{212}) were found to be relevant for $E2I_4$ as shown in Table 6.12. Although the analysis does not reveal if the emissions should be reduced or increased, the results described in Section 5.3.4 suggest that carbon aquatic emissions are lower compared to that of the reference state, A_4^0.

The analysis of combustion efficiency and carbon sequestration presented for EEI_4 is also valid for $E2I_4$. The consumption per capita of wood products (α_{78}), responsible in part for the accumulation of carbon in the system, seems to be *critical*, as it compensates to a certain extent the large magnitude of the resources consumed, mostly in the form of fossil fuels. Apparently, based on the results in Figure 5.4, the implementation of the pyrolysis process shows no influence on $E2I_4$. However, its significance seems to change when the process temperature is analyzed (α_{196}). As explained in Section 5.1.2, temperature plays an important role on the distribution of the pyrolysis products, namely char, liquid, and gas. A lower temperature produces more char, which in the model is considered as fertilizer, reducing the requirement for *resources* (R_4) and possibly increasing the accumulation of carbon (ΔS_4). The alteration of these two aggregated terms might be compensating for the loss of *product* (P_4) experienced when PLP alone is implemented.

6.3.1 Summation of Results

Under the current structure of the model and the parameter space considered, the 30% improvement target is not feasible for water and energy. In the case of energy, the relevance of parameters can change by lowering the improvement level, but if maintaining the present target is desirable, relaxing parameters associated with combustion efficiency or introducing other forms of power generation such as solar energy might be enough. These alternatives are not tested in the present dissertation, but will be recommended for future work.

Nitrogen

The flows related to the poultry industry are quite relevant to the eco-efficiency of the system with respect to nitrogen. Management strategies for reducing losses via ammonia volatilization might be appropriate. Air emissions from biological wastewater treatment in WWTPs is a loss of resources that affects indicator EEI_2 negatively, but the analysis shows that UST, conceived of only for households, is not enough, as there are other sources of N that contribute to the overall sewage N concentration.

The implementation of municipal sludge pyrolysis and finding alternative uses for CCP (coal combustion products) have a significant effect on the eco-efficiency of the system by

Table 6.12: Critical parameters for indicator $E2I_4$, eco-effectiveness of carbon.

Parameter identification code and description		**Units**	**Sector**[a]
α_{59}	Pervious area infiltration index	ratio	1
α_{61}	Average monthly cloudiness	percentage	1
α_{534}	Average air temperature	°C	1
α_{536}	Average latitude of the system	degrees	1
α_{60}	No. of days with >.01 inches of precipitation	events per year	1
α_{498}	Nutrient content in wet deposition	C content	1
α_{233}	Surface runoff nutrients (impervious areas)	C content	1
α_{315}	Recommended fertilization rates: crop and pasture	N content	2
α_{212}	Grassland floor nutrient content[b]	ratio	2
α_{429}	Pig feed requirements	Energy content	2
α_{409}	Live animal — poultry	C content	2
α_{432}	EGG composition	CH content[c]	2
α_{213}	Forestland floor nutrient content[b]	ratio	3
α_{131}	Forest area fertilized	percent	3
α_{345}	Wood (average softwood and hardwood)	C content	3
α_{121}	Above-ground biomass growth (no timberland forest)	$\mathrm{t\,ha^{-1}\,y^{-1}}$	3
α_{123}	below-ground/above-ground biomass (forests)	ratio	3
α_{360}	Paper and paperboard	C content	3
α_{78}	Timber products consumption per capita per year	$\mathrm{m^3\,y^{-1}}$	3
α_{82}	Fraction of sawmill residue used as fuel	ratio	3
α_{205}	Internal combustion efficiency for engines	ratio	4
α_{167}	Coal power plant energy efficiency	ratio	4
α_{182}	Industrial energy supplied by biomass	ratio	4
α_{447}	Natural gas composition — dry basis	Energy content	4
α_{196}	Pyrolysis process temperature	°C	5
α_{478}	O horizon layer in undisturbed forests	C content	23
α_{140}	Carbon leaching factor	ratio	23

[a] Sector are categorized as (1) water, (2) food, (3) forestry, (4) energy, (5) waste management, and (23) for those parameters associated with more than one sector.
[b] With respect to an undisturbed forest.
[c] CH carbohydrates.

preventing nutrients from being sent to landfills. Similarly, nitrogen emissions from coal and natural gas associated with power generation and other uses are found to be *critical*.

The control of surface runoff from pervious areas and nutrient content (N and P) in leachate from forests and grassland are *critical* for improving the health of the aquatic emissions. However, the opposite is true in the case of carbon, where the large availability of organic carbon in undisturbed forest floor makes the aquatic emission of the reference state larger than that obtained from the simulated case study. Therefore, the accumulation of organic material in the watershed floor is relevant to meet a level of carbon aquatic emission equivalent to the reference state.

Phosphorus

Similar to nitrogen, the eco-efficiency of the system is related, to a great extent, to the poultry industry, but the emphasis is on managing poultry litter as a product, instead of worrying about losses through volatilization (that do not take place). Sawmill efficiency also contributes to increasing the amount of P that exits the system as a product (wood in this case); therefore its effect is comparable to that of keeping poultry litter as a product. analogously, maintaining CCP and paper flows in the form of *products* are key for improving phosphorus indicators.

With respect to the health of P emissions to the atmosphere, coal combustion is the only parameter that can be controlled; thus, it is *critical* for the improvement of the system's performance in this aspect (HAE_3).

The technologies of urine separation (UST) and municipal sludge pyrolysis (MSP) are key for target attainment in terms of eco-effectiveness. Poultry litter pyrolysis (PLP) implementation, on the other hand, has the inverse effect, so a low implementation is desirable.

Carbon

The critical parameters associated with carbon have a strong connection to the energy sector, specifically to the emissions derived from fossil fuel combustion. Efficiency of gasoline combustion seems to be *critical*, but in the case of coal, because of the existence of a parameter related to the capacity of coal-fired power generation, the resulting recommendation is to avoid this energy source.

Keeping poultry manure and waste paper recovery as the flow of *products* is relevant to improving the eco-efficiency of the system in terms of carbon (EEI_4).

Carbon sequestration in forest biomass, above-ground and below-ground, and soil organic matter are key to reversing the typically outgoing emissions of carbon from urban areas into an incoming flow, as is the case for forests (the reference state). The consumption of wood materials and the conversion of sludge into fertilizer by low temperature pyrolysis act as an indirect carbon sequestration with a similar positive benefit for the improvement of the system's eco-effectiveness as reported by $E2I_4$. Along the same line, using wood as a fuel, specifically sawmill residue in the case of the UCW, worsens the air emission component of eco-effectiveness (HAE_4).

General Comments

Efforts were made to explain why parameters are *critical*, or *redundant*, but it is important to acknowledge that establishing a clear connection between some parameters and the indicator under analysis is sometimes challenging. For this reason there are a few parameters that are not included in the analysis.

The RSA method reveals whether a parameter is *critical* or *redundant*, but a high understanding of the system is required in order to generate a recommendation with respect to the management or control strategy for a parameter. In other words, knowledge of the system process units interactions is required to understand in which direction the management strategy should modify the parameter to obtain an improvement of the system's performance. Additionally, the methodology employed for this case study, i.e., testing all parameters simultaneously, does not offer explicit information about how many of the *critical* parameters should be manipulated, at a single time, to attain the stipulated target for an specific indicator. Testing each parameter separately might help to establish their individual relevance, but the scope of this exercise is to offer a general screening of the parameters that can serve as the input for a more detailed analysis.

The information generated by this kind of analysis offers researchers hints on which areas of study are possibly important to attain sustainable flows. For example, reducing the losses of nitrogen in biological wastewater treatment by recovering nitrogen from all sources, not only urine, is something that might be worth of investigating. What are the other sources of nitrogen in sewage? Is it possible to recover this nitrogen before it is discharged to the sewer network? Also, it is desirable to address those key parameters that are subject to large levels of uncertainty for two reasons: (i) if their uncertainty is reduced, the parameter might turn out to be not that *critical*, (ii) if after a better specification of the parameter range (reducing its uncertainty) it remains *critical*, then the possible benefits of manipulating the parameter value (by implementing a technical solution or adopting a new management strategy) are better assessed. In other words, the benefit measured in terms of indicator performance can be estimated more accurately. In the particular case of the Upper Chattahoochee Watershed (UCW), the concentration of surface runoff from impervious areas (mainly urban) was reported as a *critical* aspect for all nutrient species. The uncertainty level of the parameters associated with surface runoff from impervious areas is high, ranging from 3 to 5 based on the categorization specified in Table 3.12. This suggests that additional efforts are needed to establish a more accurate range of concentration applicable to the UCW.

The triplet of case studies presented in Chapters 4, 5, and the present chapter, has the purpose of revealing the practicalities of using MSA in a real life case and generating additional insight on the capabilities of the model. The conclusions drawn from this experience, together with the knowledge gained by putting together the MSA framework, are summarized in the next chapter.

Chapter 7

CONCLUSIONS AND FINAL REMARKS

"A designer knows he has achieved perfection not when there is nothing left to add, but when there is nothing left to take away." Antoine de Saint-Exupéry

7.1 Conclusions

7.1.1 The MSA Framework

A Multi-Sectoral Analysis framework that includes five industrial sectors (water, forestry, food, energy, and waste management) was developed. Besides providing information about the system based on the flows of nutrients (nitrogen, phosphorus, and carbon), water, and energy the framework makes possible the implementation of a methodology for sustainability assessment supported by the development of sustainability measures (indicators) and the incorporation of Regionalized Sensitivity Analysis (RSA). A total of eight indicators were designed to capture eco-efficiency and eco-effectiveness concepts. Those indicators under the latter concept rely on the comparison of the actual state of the system with a reference state, defined for the purposes of this dissertation as an undisturbed forest. From the experience gained throughout this dissertation, it has been demonstrated that the MSA can offer help to decision-makers and researchers in three different areas:

(i) Accounting for materials and energy. This not only offers the quantitative basis for comparison to other systems and, for instance, to learn what the other system is doing better, but also provides information about which flows, processes, and sectors of the system are the most relevant in terms of magnitude, and within which areas of the system is most of the accumulation taking place. This is valuable information for proper resource management. The Monte Carlo simulation used for sampling the parameter space enhances the results by providing information about the variability of the magnitudes of flows.

(ii) Assessment of sustainability performance. The availability of sustainability measures (the indicators) makes possible the assessment of the system *as is*, and allows compararisons of different scenarios in terms of the performance of the indicators. To the best of current knowledge, this dissertation is the first attempt to instrument the eco-effectiveness concepts in the form of quantitative measures. The analysis proposed within the MSA allows the practitioner to find trade-offs among species (materials and energy) and sectors that would remain hidden otherwise. The uncertainty associated with the MSA framework, as in any complex and data-rich systems analysis, is not disregarded.

(iii) Assessment of the feasibility of sustainability targets and which elements in the system are *critical* to attain these targets, which is particularly difficult for complex systems. The application of the RSA procedure to the MSA framework provides information that be used by researchers to orient their investigation towards areas that have regional relevance, and by decision-makers to propose reachable targets or find ways to improve their chances for reaching more speculative goals.

The capabilities of the MSA are illustrated using a case study applied to the Upper Chattahoochee Watershed. The structure of the multi-sectoral model is very general, so that in principle, the MSA can be applied to any system. The parameters can turn flows and processes "on" and "off" and adjust the activity of the different unit operations within any of the sectors, adapting in this way the model to the specific characteristics of the system.

This includes the ability that the practitioner has to manipulate the weighting parameters in Equation (3.12) to describe public desire or regional importance of one indicator over the others during the construction of the eco-effective indicator $E2I_k$. Additionally, because the framework is supported by a modeling structure, built in MATLAB®, MSA is a flexible, adaptable, and, overall, a powerful tool for systems analysis.

The framework developed only accounts for the {*environmental benignity*} component of the *triple-bottom line*, although it is important to acknowledge that the other two components, {*social legitimacy*} and {*economic feasibility*}, have a real significance for decision making. Often, environmental analysis is performed to provide information on decisions that have been already made (Hertwich *et al.*, 2000). Of the technologies screened in Chapter 5, UST is the one that interacts more with the general public; therefore requiring more analysis of the social implications of its implementation and use. This is recognized in the work performed by Lienert and Larsen (2006). At a different level, and in the particular case of MSA as part of a modeling tool, as presented herein, stakeholder involvement in environmental sustainability decisions is relevant, if not vital. In order to generate a more productive analysis of the system, decisions on which species is of regional importance or what structural changes (in the form of new technological or management strategies) should be tested requires the participation of stakeholders. Osidele (2001) recognizes this and recommends the involvement of stakeholders as early as the model development stage. In that respect, the current MSA framework serves as a template that can be tailored, thanks to its flexibility and adaptability, to the specific requirements of the prospective new case study.

When revisiting the specific scenarios explored in Chapter 5, there is not much that can be said about the economic elements associated with the technologies other than the possible complexity of implementing a decentralized technology such as UST (e.g. separation device installation, retrofitting and piping, maintenance, etc), in comparison with centralized alternatives, i.e. pyrolysis of municipal sludge (MSP) and poultry litter (PLP). In decision-making, it is more than often the case that environmental analysis is applied to advise about decisions that have been already taken (Hertwich *et al.*, 2000), but if an assessment tool provides also information of the potential economic benefit or disadvantage of adopting one or another environmental sustainability strategy, then one could say that the tool has improved the decision.

7.1.2 The Upper Chattahoochee Watershed Case

The conclusions drawn from the specific case study illustrated with the Upper Chattahoochee Watershed (UCW) are separated into the three areas of application enumerated in Section 7.1.1.

Flows of Materials and Energy

As the result of the analysis of the system *as is*, i.e., the *base case*, it was found that precipitation $147.2\,\mathrm{m^3\,s^{-1}}$ and evapotranspiration are the largest flows of water in the system, and the drivers of the water cycle within the UCW. The surface runoff produced from precipitation is about $15.3\,\mathrm{m^3\,s^{-1}}$. The largest flow generated by human intervention is for cooling in power generation processes ($18.3\,\mathrm{m^3\,s^{-1}}$), while public supply withdraws $8.8\,\mathrm{m^3\,s^{-1}}$, of which 56% is for residential use.

The major flows for nitrogen, on the other hand, are associated with imported feed for livestock ($27\,800\,\mathrm{t\,N\,y^{-1}}$) and emissions from fuel use for purposes other than power generation ($27\,000\,\mathrm{t\,N\,y^{-1}}$). Emissions from power generation (coal and natural gas) are not negligible, amounting to some $20\,000\,\mathrm{t\,N\,y^{-1}}$. The total mass of N in urine produced by the population is nearly $5000\,\mathrm{t\,N\,y^{-1}}$. Surface runoff accounts for the loss of $3600\,\mathrm{t\,N\,y^{-1}}$.

In the case of phosphorus, the largest flows are related to fodder $6000\,\mathrm{t\,P\,y^{-1}}$, mostly for the poultry industry, and nutrient application to soil $3600\,\mathrm{t\,P\,y^{-1}}$. Coal imports a significant amount of P into the system, which ends up in the form of coal combustion products (CCP) totaling nearly 2000 $\mathrm{t\,P\,y^{-1}}$, the same as the amount recovered in digested municipal sludge. Urine contributes with 500 $\mathrm{t\,P\,y^{-1}}$ of that P present in sludge.

Because the UCW generates only 10% of its power requirements, the largest flow of carbon is represented by the emissions from local fuel consumption $3.5 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, of which 60% is for transportation purposes. Imports of wood products are almost $1.0 \times 10^6\,\mathrm{t\,C\,y^{-1}}$, while the carbon sequestered in biomass is $0.6 \times 10^6\,\mathrm{t\,C\,y^{-1}}$.

Similar to water, energy is dominated by natural flows — sunlight — that are clearly much larger that any anthropogenic flow. The total requirement of energy, for human purposes, for all uses is 3% of the solar input that reaches the UCW, $3.7 \times 10^6\,\mathrm{GWh\,y^{-1}}$. After that, fuels and wood products are the most relevant flow with a magnitude of $55 \times 10^3\,\mathrm{GWh\,y^{-1}}$ (gasoline, coal, and natural gas) and about $18 \times 10^3\,\mathrm{GWh\,y^{-1}}$ (wood products and firewood). Table 4.10 reveals that there are several opportunities to take advantage of the energy that enters the system originally as solar energy, such as the heat accumulated in surfaces during the daylight period, or the energy lost by evaporation.

In summary, the interconnection between species along the five sectors is clear. For instance, carbon and energy are closely related due to the use of fuels and biomass. N and P are dominated by the poultry industry, so there is the potential for this industry to play a relevant role in the management of nutrients. Nitrogen and carbon are both related to power generation (because of the use of coal and natural gas). On the other hand, nature dominates the water and energy cycles, in consonance with the difficulties shown by the technologies tested to improve the indicators for water and energy. The system acts as a sink for all nutrient species (N, P, and C), mostly in the form of fertilizer applied to soil and wood products. Within the boundaries of the system, water is not accumulated, and although the model reports a large amount of energy stored as heat, this is only a measure of the heat stored during daytime, since most of this is lost during the night. A small amount of energy might be accumulated, but it is not quantifiable by the equations part of the model. Studies in Japan report a temperature increase of 3.1°C in Tokyo, compared to 0.6°C measured for a non-urbanized island (Hachijo), in the last 100 years (Fujibe, 2009).

Sustainability Performance Assessment

The sustainability measures are used to quantify the level of eco-efficiency and eco-effectiveness of the system under different conditions. The *base case* scenario shows that for water the system is highly efficient, since most of the water withdrawn is returned to a water source (i.e. not lost via evaporation for instance), while in terms of eco-effectiveness, the system is not too far from the reference state. In terms of nitrogen, the UCW is not wasteful but it exhibits a low productivity, 10–20%. Aquatic emissions are actually lower than what the reference state dictates, but air emissions are extremely high, far from being eco-effective. Phosphorus scores better in respect of productivity (20–40%), given that a significant amount of phosphorus is recovered as a *product* in the form of poultry litter. Due to the minimal generation of atmospheric emissions of phosphorus (coal combustion) compared to the amount received as deposition, the system is more eco-efficient in terms of P than in N. Carbon, on the other hand, shows a very low productivity: a large amount enters the system as fuel and wood products compared to the amount produced as meat and wood, for instance. About 50–80% of the carbon that enters the system as *resources* is lost as an emission (air and aquatic). Eco-efficiency and eco-effectiveness are low due to the large magnitude of air emissions and low productivity. The energy indicators associated with air emissions are marginally affected due to the influence of natural flows, but the lack of utilization of solar energy is reflected in the very low productivity, echoing the performance for carbon.

Three technologies where assessed and compared to the *base case*: urine separation (UST), municipal sludge pyrolysis (MSP), and poultry litter pyrolysis (PLP). A total of eight scenarios were evaluated to account for different combinations of the technologies. However, given that the technologies do not manipulate significant amount of water and energy, at the watershed scale, they showed little influence on those indicators related to water and energy, which are dominated by climatic conditions and natural flows. In terms of N and P, keeping the flow of poultry litter as a *product* is important to prevent indicators from worsening. The performance with respect to N is best improved by the implementation of UST and MSP together for recovering N that will otherwise be lost in the form of air emissions and landfilled material. UST alone does not score that well, because its effect is mostly translated into a more or less 40% reduction of N losses from biological wastewater treatment, which is small when compared to the magnitude of the air emissions from fuel use. However, MSP recovers N, although less N in magnitude than UST, from a smaller stream (material to landfill), showing then a larger improvement. The situation is different for phosphorus, where the best technology is featured by MSP alone. P is not lost in wastewater treatment plant (WWTP) emissions and UST would recover roughly 25% of all the P sent to WWTPs, compared to nearly 100% in MSP. The flows of carbon are tightly related to the flows of wood and fuel. The former is not manipulated by the technologies, while the pyrolysis process, although it does contribute for the latter, is negligible compared to the flows of fossil fuels. For this reason, the technologies have no apparent influence on those indicators that reflect the system's performance with respect to carbon. In order to generate a significant improvement of the indicators associated with air emissions of carbon and nitrogen, it is necessary to address the emissions from fossil fuel combustion, as was demonstrated by a pseudo scenario, described in Section 5.3.5, where power plant emissions are harvested and converted them into a useful product. This is corroborated by the implementation of the RSA procedure for identifying those key aspects of the MSA model for improvement (see below).

Although the analysis of the case study presented in this dissertation is made as comprehensive as possible, i.e., by examining all indicators and all species considered in the MSA framework, the practitioner has the flexibility to choose any species and indicator of interest. In this way, the analysis can be tailored for the investigation of issues that are related to a specific area. For instance, if the region is a coastal area where there is public concern about eutrophication due to high concentrations of nitrogen species, the practitioner might focus on analyzing those indicators associated with aquatic emissions: EEI_2, HWE_2, and $E2I_2$.

Critical Elements to achieve Targets

The previous section evaluates the system using a forward approach, i.e., adjust the system first and then observe the improvements, while the application of the RSA procedure within the MSA framework is an inverse analysis in the sense that targets are set and then the system is studied with the hope of identifying the elements of the system that are key to achieving those goals. A total of eleven indicators were selected for this exercise and a nominal improvement of 30% is proposed for them.

The results showed that the level of improvement is not attainable in the case of water and energy. The former because it is already close to the maximum possible efficiency and eco-effectiveness, but for the latter, it has to do with the fact that the system, in its current structure, depends on fuels that enter the system and leave as emissions and the efficiency parameters of energy (fuel) utilization are not flexible enough to provoke a significant improvement. In other words, a 100% efficient internal combustion engine might bring a noticeable change in the performance.

The food sector, represented mainly by the poultry industry, exhibits the largest participation in terms of the number of *critical* parameters, followed by the water, forestry, and energy sectors. This suggests that the food sector is key for improving the system by 30% in terms of nitrogen, phosphorus, and carbon. The parameters found to be *critical* for the most number of indicators at the same time, five in total, were mostly those associated with climatic conditions and soil infiltration. It was found that the importance of the former group is because of their indirect relation — via precipitation and evaporation — with impervious surface runoff, which was identified to be *critical* for almost all measures, as shown in Table 7.1, which summarizes the important aspects that must be taken into consideration for improving the system. In the particular case study of the UCW, Table 7.1 condenses the results discussed in Chapter 6 into a form that can be presented to decision-makers for a first screening of possible opportunities for improvement.

7.2 Recommendations for Future Work

The application of Substance Flow Analysis (SFA) of nutrients, water, and energy within a multi-sectoral approach, together with eco-effectiveness concepts, was presented in this dissertation as the MSA framework, which must be seen as a first step that needs further development. The following list describes possible future work that can improve or complement the MSA framework.

(1) Presently, the MSA framework has been tested only for the UCW. The next logical step, therefore, is to expand the application of it to other regions with different characteristics (e.g. developing countries) in terms of climate, consumption of resources, and economic activities. This involves data collection associated with the new system, possibly followed by the adaptation of the model structure to include processes or infrastructures that are not present in the UCW.

(2) Based on the discussion in Section 7.1.1 about the importance of the *triple-bottom line* in assessment tools, it seems imperative to recommend the expansion of the current MSA framework to include aspects of {*social legitimacy*} and {*economic feasibility*}. Advancing on this front will enable MSA as a tool for comprehensive analyses, with capabilities to explore the trade-offs not only at the environmental level. Since the MSA

Table 7.1: Summary of critical aspects of the Upper Chattahoochee Watershed.

Aspect of the MSA	**Indicators**								
	EEI_2	HWE_2	$E2I_2$	EEI_3	HWE_3	$E2I_3$	EEI_4	HAE_4	$E2I_4$
Runoff from impervious areas	x	x	x	x	x	x			x
Emissions from coal combustion			x			x	x	x	x
Poultry litter as a product	x			x		x	x		
Emissions from natural gas combustion	x		x						x
Alternative uses for Coal Combustion Products			x	x	x				
Leaching of nutrients from forests		x			x				x
Wood productivity described by sawmill efficiency				x				x	x
Emissions from gasoline							x	x	x
N fixation in forests		x	x						
Leaching of nutrients from grassland		x							x
Paper recovery and recycling				x					x
Sources of P to sewage				x	x				
Municipal sludge pyrolysis					x	x			
Fuel consumption for transportation							x	x	
Carbon sequestration in forests								x	x
Emissions of N from biological wastewater treatment	x								
Leaching of nutrients from cropland						x			
Urine separation technology						x			
Fuel consumption for industrial use							x		
Composting of food waste								x	
Pyrolysis process temperature									x

framework makes use of Substance Flow Analysis (SFA) as its core methodology, the approach for instrumenting the social and economic components must include methods that posses a similar systems analysis perspective.

(3) In connection with the foregoing recommendation (2), economic aspects such as the monetary value of materials will allow the practitioner to differentiate the various forms for the same specie. For instance, nitrogen in inorganic fertilizer is more valuable than nitrogen in poultry litter, and this is more valuable than the nitrogen found in coal. This approach might be helpful for addressing the over penalization of the indicators that took place in Chapter 5 when removing poultry litter from the *product* flow for generating possibly more valuable products from the pyrolysis process.

(4) As discussed in Section 3.6, further analysis of those parameters identified as *critical* is possible by implementing the Tree-Structured Density Estimation (TSDE) method. This will complement the results in Chapter 6 by determining the $\{B\}$ parameter combinations that team together to match the *behavior* and by establishing the relative importance of each parameter in a tree-like hierarchical histogram. TSDE has been successfully used in other studies related to non-point source sediment and nutrient management (Arabi *et al.*, 2007), global carbon cycling models (Grieb *et al.*, 1999), and with emphasis on interconnecting stakeholder knowledge and model simulation and forecasting (Osidele, 2001).

(5) By incorporating transient functions that describe how the system's characteristics vary in time, such as population, land use, consumption of resources, and production, it would be possible to explore how the order and the timing of implementation of technological solutions affect the system's behavior and performance. A transient model would have the capability of exploring the effects of infrastructure transitions (steps of structural change). This feature can be exploited also with an inverse approach, that is, test the parameter space for incremental levels of performance improvement, e.g. 10, 20, 30, 40,

and 50%, and investigate how this is reflected in the number of *critical* elements of the system. One would expect that for a lower improvement level, a larger group of behavior-giving parameters will be reported.

(6) Complementing recommendation (5), further disaggregating some of the individual processes, e.g., household wastewater from industrial and commercial uses, will make it possible to test a much larger number of technological solutions, or at least allow more manipulation of flows and processes. In a similar spirit, differentiating the various chemical forms of materials, e.g. N_2O from N_2 or CO_2 from CH_4, can make more specific the way flows are classified. The difficulty with this recommendation is that more data will be required with the consequent addition of uncertainty and model complexity.

(7) Excepting for the case of evapotranspiration, ambient temperature was not considered for processes or parameters that are known to be influenced by climate, such as nitrogen volatilization and denitrification, energy usage, water consumption, and wastewater treatment processes. Although the uncertainty ranges assigned to parameters might cover part of the influence of climate change, a more explicit description of the effects of temperature could expand the applicability of the MSA framework to climate change studies.

(8) Although the results, derived from the analysis of indicators, reported for the UCW provided vast amounts of information, it is acknowledged that more efforts are needed to improve the formulation of the sustainability indicators proposed in this dissertation. The mathematical behavior of these is still complex, as shown in Appendix E. This translates into extensive work for the interpretation of results and the definition of targets, both subject to the behavior of indicators. In any case, indicators must include concepts of eco-effectiveness and take into account that the emissions defined for the reference state, A_k^0 and E_k^0, are flows that can change their direction (sign), particularly with respect to nitrogen.

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Appendix A

List of Abbreviations and Symbols

Abbreviations

A	Area
BOD	Biochemical Oxygen Demand
C	Carbon
CO	Comercial
COD	Chemical Oxygen Demand
D	Water Discharges
DE	Digestible Energy
DO	Domestic or residential
DOM	Dead organic matter
E2I	Indicator: eco-effectiveness
EEI	Indicator: eco-efficiency, products to emissions
EIA	Energy Information Agency
EIA	Environmental impact assessment
EMS	Environmental management systems
GHG	Green House Gases
HAE	Indicator: degree of health of air emissions
HWE	Indicator: degree of health of water emissions
IBT	Inter-basing transfer (water or wastewater)
IN	Industrial

LCA	Life Cycle Assessment
LCA	life-cycle assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventories
MFA	Material Flow Analysis
MSA	Multi-sectoral System Analysis
MSW	Municipal Solid Waste
N	Nitrogen
NG	Natural gas
NPDES	National Pollutant Discharge Elimination System
P	Phosphorus
PG	Power generation
PRI	Indicator: products to resources
PWI	Indicator: products to wastes
PU	Public (with respect to water or energy use)
RA	risk assessment
RWI	Indicator: resources to wastes
SFA	Substance Flow Analysis
TA	technology assessment
TC	Total Carbon as C
TIC	Total Inorganic Carbon
TIN	Total Inorganic Nitrogen
TKN	Total Kjeldahl Nitrogen
TN	Total nitrogen as N
TOC	Total Organic Carbon
TP	Total Phosphorus as P

UCW	The Upper Chattahoochee Watershed
UMA	Urban Material Analysis
US	The United States of America
WEF	Indicator: waste equals food
WMS	Waste Management Sector
WWTP	Wastewater Treatment Plant

Symbols

α	Emprirical parameter for calculating Q_H and Q_E
α_j	The jth parameter of the MSA model
$\beta 1_k$	Aggregation term for indicator E2I
$\beta 2_k$	Aggregation term for indicator E2I
$\beta 3_k$	Aggregation term for indicator E2I
β	Emprirical parameter for calculating Q_H and Q_E
ΔC	Change in carbon stock in biomass (plants)
ΔQ_S	Net heat storage
ΔS_k	Accumulation term of the kth species
λ_w	Water heat of vaporization, i.e. $1.0\,\mathrm{kcal\,kg^{-1}}$
$\overline{\alpha}_j$	Most likely value of the jth parameter
ρ	Population per acre
A_j	Pre-exponential constant of the jth phase (L, S, G), s^{-1}
A_k^0	Healthy water emission of the kth species
C_{fract}	Mass fraction of carbon (typically 0.4–0.5)
C_k^j	Concentration of kth species in the jth flow
E_k^0	Healthy air emission of the kth species
M_p	Precipitation at which $E_{t,a} \rightarrow E_{t,p}$

A_k	Emissions to aquatic bodies of the kth species
B_w	Body mass
$E_{t,a}$	Actual Evapotranspiration
$E_{t,p}$	Potential Evapotranspiration
E_c	Export coefficient
E_j	Activation Energy of reaction of the jth phase (L, S, G), $\mathrm{kJ\,mol^{-1}}$
E_k	Emissions to atmosphere of the kth species
F_k^j	Flow of the kth species as part of the jth flow
G	Pyrolysis product - gas phase
G_w	Average annual above-ground biomass growth
H_B	Energy content of the pyrolysis feed flow
H_G	Energy content of the pyrolysis gaseous product
H_L	Energy content of the pyrolysis liquid product
H_S	Energy content of the pyrolysis solid product
I_k	Generic indicator of the kth species
I_k^{imp}	Improved value of a generic indicator of the kth species
I_w	Interbasin transfer: water
$I_w w$	Interbasin transfer: wastewater
k_{global}	Global reaction rate of the pyrolysis process
k_j	Kinetic rate constant of the jth phase (L, S, G), $\mathrm{s^{-1}}$
L	Pyrolysis product - liquid phase
M	Metabolic rate of an organism
$M_{consumed}$	Amount of material consumed within the system
M_{ie}	Material imported (positive value) or exported (negative value)
$M_{produced}$	Material produced within the system
M_R	Metabolic respiration in $\mathrm{kg\,C\,y^{-1}}$

M_E	Mass of water evaporated
M_f	Soil moisture correction factor
N_{input}	Nutrient input to soil
P_k	Products of the kth species
Q^*	Net all-wave radiation
Q_{LW}	Net long wave radiation
Q_{SR}	Solar radiation received on a horizontal plane
Q_E	Latent heat flux lost due to evaporation and transpiration
Q_H	Turbulent sensible heat flux from the ground surface
R	Universal gas constant, $8.31 \times 10^{-3}\,\mathrm{KJ\,mol^{-1}\,K^{-1}}$
R_{ab}	Ratio of below-ground to above-ground biomass
R_k	Resources of the kth species
R_{losses}	Nutrient losses in runoff in $\mathrm{kg\,ha^{-1}}$
R_o	Rapid Surface Runoff
S	Pyrolysis product - solid phase
S_i	Soil infiltration
T	Reaction temperature in Arrhenius Equation, K
u_j	Uncertainty factor of the jth parameter
W_i	Withdrawals
W_k	Wastes of the kth species
W_{precip}	Precipitation
Y_G	Yield coefficients of the gas phase in the pyrolysis process
Y_L	Yield coefficients of the liquid phase in the pyrolysis process
Y_S	Yield coefficients of the solid phase in the pyrolysis process
CH_4	Methane
CO	Carbon Oxide

CO_2	Carbon dioxide
H_2O	Water
N_2O	Nitrous Oxide
NH_x	Ammonia plus ammonium
NH_3	Ammonia
NH_4	Ammonium
NO_x	Nitrogen Oxide(s)
NO_2	Nitrite
NO_3	Nitrate
PO_4	Phosphate
P_2O_5	Phosphorus Oxide

Appendix B

List of Parameters and Inputs

The following is a full list of the parameters used by the computational platform of the Multi-sectoral Systems Analysis (MSA). Those parameters that are not described are empty slots for future parameters.

ID	Description
α_1	Population growth constant, 1/y
α_2	Per Capita DO water use (served by Public Supply), gpd/cap
α_3	Ratio of DO self supplied population (SS pop / total pop), ratio
α_4	Radio of self-supplied DO water from GW, ratio
α_5	Ratio of DO consumptive water use - mainly garden, ratio
α_6	Per capita total CO water use (total area population), gpd/cap
α_7	Ratio of CO self supplied (water SS / water total), ratio
α_8	Radio of self-supplied CO water from GW, ratio
α_9	Ratio of CO consumptive water use (Consumptive/Total), ratio
α_{10}	Per capita public water use (total area population), gpd/cap
α_{11}	Ratio of public losses, ratio
α_{12}	Per capita total industrial water use (total area population), gpd/cap
α_{13}	Ratio of industry discharge (dis. to water source / total industry), ratio
α_{14}	Ratio of IN self supplied (water SS / water total), ratio
α_{15}	Radio of self-supplied IN water from GW, ratio
α_{16}	Ratio of IN consumptive use (Consumptive/total), ratio
α_{17}	Change rate for mining water use, Mgal per d/y
α_{18}	Ratio of MI water use from GW, ratio
α_{19}	Ratio of MI consumptive use (consumptive/total), ratio
α_{20}	Ratio of LI water use from GW, ratio
α_{21}	Ratio of LI consumptive use (consumptive/total), ratio
α_{22}	Water use for cattle and calves operations, gpd/head
α_{23}	Water use for poultry operations, gpd/head
α_{24}	Water use for pigs and hogs operations, gpd/head
α_{25}	Cattle Annual inventory growth rate, head/head

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ID	Description
α_{26}	Poultry Annual inventory growth rate, head/head
α_{27}	Hogs and pigs Annual inventory growth rate, head/head
α_{28}	Water withdrawals for power generation - Coal , gal/kWh
α_{29}	Water withdrawals for power generation - NG, gal/kWh
α_{30}	Water withdrawals for power generation - Nuclear, gal/kWh
α_{31}	Water withdrawals for power generation - Diesel, gal/kWh
α_{32}	Water withdrawals for power generation - Alternative p1, gal/kWh
α_{33}	Water withdrawals for power generation - Alternative p2, gal/kWh
α_{34}	Water withdrawals for power generation - Alternative p3, gal/kWh
α_{35}	Consumptive water use for power generation - Coal, gal/kWh
α_{36}	Consumptive water use for power generation - NG, gal/kWh
α_{37}	Consumptive water use for power generation - Nuclear, gal/kWh
α_{38}	Consumptive water use for power generation - Diesel, gal/kWh
α_{39}	Consumptive water use for power generation - Alternative p1, gal/kWh
α_{40}	Consumptive water use for power generation - Alternative p2, gal/kWh
α_{41}	Consumptive water use for power generation - Alternative p3, gal/kWh
α_{42}	Power generation water use from GW, ratio
α_{43}	Water withdrawals for fuel production - Alternative f1, gal w/gal fuel
α_{44}	Water withdrawals for fuel production - Alternative f2, gal w/gal fuel
α_{45}	Water withdrawals for fuel production - Alternative f3, gal w/gal fuel
α_{46}	Consumptive water use for fuel production - Alternative f1, gal w/gal fuel
α_{47}	Consumptive water use for fuel production - Alternative f2, gal w/gal fuel
α_{48}	Consumptive water use for fuel production - Alternative f3, gal w/gal fuel
α_{49}	Fuel production water use from GW, ratio
α_{50}	Fraction of irrigated crops, ratio
α_{51}	Irrigation rate for crops, m/y
α_{52}	Irrigation rate for recreational areas, m/y
α_{53}	Fraction of irrigation water from GW, ratio
α_{54}	Sewer inflow portion of runoff, ratio
α_{55}	Sewer infiltration index, ratio
α_{56}	Impervious Area Retention volume, mm
α_{57}	Effective Impervious Areas (that produces runoff), ratio
α_{58}	Ratio of GW over the total withdrawal for public supply, ratio
α_{59}	Pervious area infiltration index, ratio
α_{60}	Number of Days with Precipitation ¿.01 inch, No. events per y
α_{61}	Average monthly cloudiness, percentage
α_{62}	Soil average Clay content (within 0–25 cm depth), percentage
α_{63}	Soil average Sand content (within 0–25 cm depth), percentage
α_{64}	Watershed relief (highest - lowest elevation), m
α_{65}	Logging residue sent to biofuel production, ratio
α_{66}	Softwood - Live trees average net annual growth, m3/ha*y
α_{67}	Hardwood - Live trees average net annual growth, m3/ha*y

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ID	Description
α_{68}	Softwood - Live trees average annual removal, m3/ha*y
α_{69}	Hardwood - Live trees average annual removal, m3/ha*y
α_{70}	Softwood - Output of roundwood products, ratio v/v
α_{71}	Hardwood - Output of roundwood products, ratio v/v
α_{72}	Softwood logging residue, ratio v/v
α_{73}	Hardwood logging residue, ratio v/v
α_{74}	Sawmill efficiency - lumber yield, ratio v/v
α_{75}	Sawmill efficiency - bark yield, ratio v/v
α_{76}	Sawmill efficiency - Coarse residue, ratio v/v
α_{77}	Sawmill efficiency - Fine residue, ratio v/v
α_{78}	Timber products consumption per capita per yearnt), m3 per cap/y
α_{79}	Firewood consumption per capita per year, m3 per cap/y
α_{80}	Use of Paper/Paperboard per capita, m3 per cap/y
α_{81}	Maximum fraction of sawmill residue locally used, ratio
α_{82}	Fraction of sawmill residue used as fuel, ratio
α_{83}	Fraction of sawmill residue used for other products, ratio
α_{84}	MSW disposal per capita, kg per cap/d
α_{85}	MSW paper disposal factor, ratio
α_{86}	MSW food disposal factor, ratio
α_{87}	MSW wood disposal factor, ratio
α_{88}	MSW yard waste disposal factor, ratio
α_{89}	Paper/Paperboard recovery factor, ratio
α_{90}	Food recovery factor, ratio
α_{91}	Wood recovery factor (as a function of generation), ratio
α_{92}	Yard waste recovery factor (as a function of generation), ratio
α_{93}	Disposed MSW to incineration, ratio
α_{94}	Disposed MSW to landilling, ratio
α_{95}	Urine production factor (wet basis), kg per cap/d
α_{96}	Urine Moisture content, ratio
α_{97}	Efficiency of urine separation device, ratio
α_{98}	Urine Separation implementation ratio (on a person basis), ratio
α_{99}	Faeces production factor (wet basis), kg per cap/d
α_{100}	Faeces Moisture Content, ratio
α_{101}	Faeces Separation implementation ratio, ratio
α_{102}	Carbon Emission factor for drained organic soils in forests, tonne/ha*y
α_{103}	Carbon Emission factor for drained organic soils in grassland, tonne/ha*y
α_{104}	Carbon Emission factor for drained organic soils in cropland, tonne/ha*y
α_{105}	WWTP - Plant-wide BOD5 removal rate (water phase), ratio
α_{106}	WWTP - Plant-wide Nitrogen gas N2 release rate (fraction of influent), ratio
α_{107}	WWTP - Plant-wide PHOSPHORUS removal rate (water phase), ratio
α_{108}	WWTP - Oxigen endogenous decay coefficient (ke'), day-1
α_{109}	WWTP - Oxigen yield coefficient (Yb') , mg/mg

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ID	Description
α_{110}	WWTP - Cell endogenous decay coefficient (ke) , day-1
α_{111}	WWTP - Biodegradable yield coefficient (Yb) , mg/mg
α_{112}	WWTP - Operational MLSS concentration, mg/L
α_{113}	WWTP - MLVSS/MLSS activated sludge, kg/kg
α_{114}	WWTP - reactor space loading (kg BOD/day-m3), kg/d.m3
α_{115}	,
α_{116}	WWTP - Ammonia Emission Factor (kg NH3-N / kg N sewage), kg/kg
α_{117}	WWTP - Nitrous Oxide Emission Factor (kg N2O-N / kg N sewage), kg/kg
α_{118}	WWTP - Plant-wide NITROGEN removal rate (water phase), ratio
α_{119}	Default reference soil organic Carbon stock for mineral soils, tonne/ha
α_{120}	Mortality rate (fraction of above-ground biomass growth) forests, ratio
α_{121}	Above-ground biomass growth (forests - no timberland) - d.m., tonne/ha*y
α_{122}	Above-ground biomass (forests - no timberland) - d.m., tonne/ha
α_{123}	below-ground biomass / above-ground biomass (forests) - d.m., tonne/tonne
α_{124}	Nitrogen Fixation Rate - Grassland, kg/ha.y
α_{125}	Nitrogen Fixation Rate - Forest Areas, kg/ha.y
α_{126}	Nitrogen Fixation Rate - Crop land, kg/ha.y
α_{127}	Denitrification Rate - Grassland, kg/ha.y
α_{128}	Denitrification Rate - Forest Areas, kg/ha.y
α_{129}	Denitrification Rate - Crop land, kg/ha.y
α_{130}	Percentage of Clear cut and sparse areas that is fertilized (grass), percent
α_{131}	Percentage of Forest Areas that is fertlized, percent
α_{132}	Percentage of Crop and pastures that is fertilized, percent
α_{133}	Nitrogen Volatilization from Inorganic Fertlizer (IF), kg N/kg applied
α_{134}	Nitrogen Volatilization from Sewage Sludge (SS), kg N/kg applied
α_{135}	Nitrogen Volatilization from Poultry Litter (PL), kg N/kg applied
α_{136}	Nitrogen Volatilization from other Organic Manure, kg N/kg applied
α_{137}	Yard waste and grass left on site (as a function of generation), ratio
α_{138}	Yield losses from crops (losses/Yield), ratio
α_{139}	Carbon runoff factor, ratio
α_{140}	Carbon leaching factor, ratio
α_{141}	Nitrogen leaching factor, ratio
α_{142}	Phosphorus leaching factor, ratio
α_{143}	Plant Available Nitrogen (organic material before composting), ratio
α_{144}	Plant Available Phosphorus (organic material before composting), ratio
α_{145}	Canopy cover for low intensity urban areas, percent
α_{146}	Canopy cover for high intensity urban areas, percent
α_{147}	Fraction of Logging Residue left onsite, ratio
α_{148}	Impervious Area in High Intensity urban Areas, percent
α_{149}	Fruit consumption, kg per cap/y
α_{150}	Cereal consumption, kg per cap/y
α_{151}	Vegetables consumption, kg per cap/y

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ID	Description
α_{152}	Bovine meat consumption, kg per cap/y
α_{153}	Poultry meat consumption, kg per cap/y
α_{154}	Pig meat consumption, kg per cap/y
α_{155}	Fish/Seafood consumption (freshwater fish, seafood), kg per cap/y
α_{156}	Dairy consumption (milk, butter/ghee, eggs, cheese), kg per cap/y
α_{157}	Others consumption (Alcoholic bev., Veg. Oil, Sugar, etc), kg per cap/y
α_{158}	Cattle selling rate (a ratio of inventory), head/head
α_{159}	Poultry selling rate (a ratio of inventory), head/head
α_{160}	Hogs and pigs selling rate (a ratio of inventory), head/head
α_{161}	Cattle manure production rate (kg manure/Body Weight kg), kg/kg.y
α_{162}	Poultry manure production rate (kg manure/Body Weight), kg/kg.y
α_{163}	Pigs manure production rate (kg manure/Body Weight), kg/kg.y
α_{164}	Maximum Fraction of Cattle Manure Used as fertilizer, ratio
α_{165}	Maximum Fraction of Poultry Manure Used as fertilizer, ratio
α_{166}	Maximum Fraction of Swine Manure Used as fertilizer, ratio
α_{167}	Coal power plant energy efficiency, ratio
α_{168}	NG power plant energy efficiency, ratio
α_{169}	Diesel power plant energy efficiency, ratio
α_{170}	Power plant energy efficiency Alternative p1 , ratio
α_{171}	Power plant energy efficiency Alternative p2, ratio
α_{172}	Power plant energy efficiency Alternative p3, ratio
α_{173}	Electricity Distribution Losses (losses/delivered), ratio
α_{174}	Residential Energy use (per Household), MWh/y.house
α_{175}	Residential Energy supplied by Natural Gas, ratio
α_{176}	Residential Energy supplied by Biomass, ratio
α_{177}	Commercial Energy Use (per capita), MWh/y.cap
α_{178}	Commercial Energy supplied by Natural Gas, ratio
α_{179}	Commercial Energy supplied by Biomass, ratio
α_{180}	Industrial Energy Use (per capita), MWh/y.cap
α_{181}	Industrial Energy supplied by Natural Gas, ratio
α_{182}	Industrial Energy supplied by Biomass, ratio
α_{183}	Industrial Energy supplied by Coal, ratio
α_{184}	Transportation Energy Use (per capita), MWh/y.cap
α_{185}	Transportation Energy supplied by Natural Gas, ratio
α_{186}	Transportation Energy supplied by Diesel, ratio
α_{187}	Transportation Energy supplied by Gasoline, ratio
α_{188}	Biofuel proportion in motor engine use - diesel, ratio
α_{189}	Biofuel proportion in power generation - diesel, ratio
α_{190}	Biofuel proportion in motor engine use - gasoline, ratio
α_{191}	MSW incineration efficiency, ratio
α_{192}	Manure Sent to Composting (after pyrolysis of poultry manure), ratio
α_{193}	Poultry manure sent to Pyrolysis, ratio

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ID	Description
α_{194}	Treated Sludge sent to Composting (after pyrolysis), ratio
α_{195}	Treated Sludge sent to Pyrolysis, ratio
α_{196}	Pyrolysis process temperature, Celsius
α_{197}	CCP sent to lanfill (the rest is exported for use), ratio
α_{198}	Fruit/Orchard yield factor, tonne/acre
α_{199}	Cereal Crop yield factor, cwt/acre
α_{200}	Veggie Crop yield factor, cwt/acre
α_{201}	Feed Crop yield factor, tonne/acre
α_{202}	Cattle Annual Breed factor (a ratio of inventory), head/head
α_{203}	Poultry Annual Breed factor (a ratio of inventory), head/head
α_{204}	Pig Annual Breed factor (a ratio of inventory), head/head
α_{205}	Internal combustion efficiency of engines (gasoline or diesel), ratio
α_{206}	Internal combustion efficiency of engines (Natural Gas), ratio
α_{207}	Household and industrial firewood combustion efficiency, ratio
α_{208}	Household and industrial natural gas combustion efficiency, ratio
α_{209}	Fraction of landfill gas used for energy recovery, ratio
α_{210}	Nitrogen runoff factor, ratio
α_{211}	Phosphorus runoff factor, ratio
α_{212}	Grassland floor nutrient content with respect to undisturbed forest, ratio
α_{213}	Forestland floor nutrient content with respect to undisturbed forest, ratio
α_{214}	Cropland floor nutrient content with respect to undisturbed forest, ratio
α_{215}	Untreated Municipal Wastewater, mg/L N
α_{216}	Untreated Municipal Wastewater, mg/L P
α_{217}	Untreated Municipal Wastewater, mg/L BOD
α_{218}	Untreated Municipal Wastewater, kWh/tonne E
α_{219}	Human Urine, % Dry Solids N
α_{220}	Human Urine, % Dry Solids P
α_{221}	Human Urine, % Dry Solids C
α_{222}	Human Urine, kWh/tonne E
α_{223}	Human Feaces, % Dry Solids N
α_{224}	Human Feaces, % Dry Solids P
α_{225}	Human Feaces, % Dry Solids C
α_{226}	Human Feaces, kWh/tonne E
α_{227}	Sludge Digester Supernatant , mg/L N
α_{228}	Sludge Digester Supernatant , mg/L P
α_{229}	Sludge Digester Supernatant , mg/L TSS
α_{230}	Sludge Digester Supernatant , - E
α_{231}	Surface Runoff nutrients (Impervious Areas), mg/L N
α_{232}	Surface Runoff nutrients (Impervious Areas), mg/L P
α_{233}	Surface Runoff nutrients (Impervious Areas), mg/L C
α_{234}	Surface Runoff nutrients (Impervious Areas), - E
α_{235}	Grassland - Background export coefficient, kg/ha N

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ID	**Description**
α_{236}	Grassland - Background export coefficient, kg/ha P
α_{237}	Grassland - Background export coefficient, kg/ha C
α_{238}	Grassland - Background export coefficient, E
α_{239}	Forestland - Background export coefficient, kg/ha N
α_{240}	Forestland - Background export coefficient, kg/ha P
α_{241}	Forestland - Background export coefficient, kg/ha C
α_{242}	Forestland - Background export coefficient, E
α_{243}	Cropland - Background export coefficient, kg/ha N
α_{244}	Cropland - Background export coefficient, kg/ha P
α_{245}	Cropland - Background export coefficient, kg/ha C
α_{246}	Cropland - Background export coefficient, E
α_{247}	,
α_{248}	,
α_{249}	,
α_{250}	,
α_{251}	,
α_{252}	,
α_{253}	,
α_{254}	,
α_{255}	,
α_{256}	,
α_{257}	,
α_{258}	,
α_{259}	,
α_{260}	,
α_{261}	,
α_{262}	,
α_{263}	,
α_{264}	,
α_{265}	,
α_{266}	,
α_{267}	,
α_{268}	,
α_{269}	,
α_{270}	,
α_{271}	,
α_{272}	,
α_{273}	,
α_{274}	,
α_{275}	,
α_{276}	,
α_{277}	,

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ID	Description
α_{278}	,
α_{279}	,
α_{280}	,
α_{281}	,
α_{282}	,
α_{283}	,
α_{284}	,
α_{285}	,
α_{286}	,
α_{287}	,
α_{288}	,
α_{289}	,
α_{290}	,
α_{291}	,
α_{292}	,
α_{293}	,
α_{294}	,
α_{295}	Surface water - reservoir (water source), mg/L N
α_{296}	Surface water - reservoir (water source), mg/L P
α_{297}	Surface water - reservoir (water source), mg/L C
α_{298}	Surface water - reservoir (water source), - E
α_{299}	,
α_{300}	,
α_{301}	,
α_{302}	,
α_{303}	Ground water - aquifers (water source), mg/L N
α_{304}	Ground water - aquifers (water source), mg/L P
α_{305}	Ground water - aquifers (water source), mg/L C
α_{306}	Ground water - aquifers (water source), - E
α_{307}	Recommended fertilization rates: Grass and lawn, kg/ha.y N
α_{308}	Recommended fertilization rates: Grass and lawn, kg/ha.y P
α_{309}	Recommended fertilization rates: Grass and lawn, C
α_{310}	Recommended fertilization rates: Grass and lawn, E
α_{311}	Recommended fertilization rates: Forest, kg/ha.y N
α_{312}	Recommended fertilization rates: Forest, kg/ha.y P
α_{313}	Recommended fertilization rates: Forest, C
α_{314}	Recommended fertilization rates: Forest, - E
α_{315}	Recommended fertilization rates: Crop and Pasture, kg/ha.y N
α_{316}	Recommended fertilization rates: Crop and Pasture, kg/ha.y P
α_{317}	Recommended fertilization rates: Crop and Pasture, C
α_{318}	Recommended fertilization rates: Crop and Pasture, E
α_{319}	N content per fresh kg of Inorganic Fertlizer (IF), % DM N

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ID	**Description**
α_{320}	P content per fresh kg of Inorganic Fertlizer (IF), % DM P
α_{321}	, % DM
α_{322}	, kWh/tonne
α_{323}	Nutrient content per fresh kg of Cattle Manure (CM), % DM N
α_{324}	Nutrient content per fresh kg of Cattle Manure (CM), % DM P
α_{325}	Nutrient content per fresh kg of Cattle Manure (CM), % DM C
α_{326}	Nutrient content per fresh kg of Cattle Manure (CM), kWh/tonne E
α_{327}	Nutrient content per fresh kg of Cattle Manure (CM), % W
α_{328}	Nutrient content of fresh Poultry Litter (PL), % DM N
α_{329}	Nutrient content of fresh Poultry Litter (PL), % DM P
α_{330}	Nutrient content of fresh Poultry Litter (PL), % DM C
α_{331}	Nutrient content of fresh Poultry Litter (PL), kWh/tonne E
α_{332}	Nutrient content of fresh Poultry Litter (PL), MC % W
α_{333}	Nutrient content per fresh kg of Swine Manure (SM), % DM N
α_{334}	Nutrient content per fresh kg of Swine Manure (SM), % DM P
α_{335}	Nutrient content per fresh kg of Swine Manure (SM), % DM C
α_{336}	Nutrient content per fresh kg of Swine Manure (SM), kWh/tonne E
α_{337}	Nutrient content per fresh kg of Swine Manure (SM), MC % W
α_{338}	Nutrient content of compost (CP), % DM N
α_{339}	Nutrient content of compost (CP), % DM P
α_{340}	Nutrient content of compost (CP), % DM C
α_{341}	Nutrient content of compost (CP), kWh/tonne E
α_{342}	Nutrient content of compost (CP), MC % W
α_{343}	Wood (average softwood and hardwood), fraction w/w N
α_{344}	Wood (average softwood and hardwood), fraction w/w P
α_{345}	Wood (average softwood and hardwood), fraction w/w C
α_{346}	Wood (average softwood and hardwood), kWh/tonne E
α_{347}	Wood (average softwood and hardwood), fraction w/w W
α_{348}	Bark, fraction w/w N
α_{349}	Bark, fraction w/w P
α_{350}	Bark, fraction w/w C
α_{351}	Bark, kWh/tonne E
α_{352}	Bark, fraction w/w W
α_{353}	Yard/Agricultural Residue , fraction w/w N
α_{354}	Yard/Agricultural Residue , fraction w/w P
α_{355}	Yard/Agricultural Residue , fraction w/w C
α_{356}	Yard/Agricultural Residue , kWh/tonne E
α_{357}	Yard/Agricultural Residue , fraction w/w W
α_{358}	Paper and Paperboard, fraction w/w N
α_{359}	Paper and Paperboard, fraction w/w P
α_{360}	Paper and Paperboard, fraction w/w C
α_{361}	Paper and Paperboard, kWh/tonne E

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Continued from previous page

ID	Description
α_{362}	Paper and Paperboard, fraction w/w W
α_{363}	Fruit, kg/kg N
α_{364}	Fruit, kg/kg P
α_{365}	Fruit, kg/kg C
α_{366}	Fruit, Kcal/kg E
α_{367}	Cereal, kg/kg N
α_{368}	Cereal, kg/kg P
α_{369}	Cereal, kg/kg C
α_{370}	Cereal, Kcal/kg E
α_{371}	Vegetables, kg/kg N
α_{372}	Vegetables, kg/kg P
α_{373}	Vegetables, kg/kg C
α_{374}	Vegetables, Kcal/kg E
α_{375}	Fish/Seafood, kg/kg N
α_{376}	Fish/Seafood, kg/kg P
α_{377}	Fish/Seafood, kg/kg C
α_{378}	Fish/Seafood, Kcal/kg E
α_{379}	Others (Alcoholic beverages, Veg. Oil, Sugar, etc), kg/kg N
α_{380}	Others (Alcoholic beverages, Veg. Oil, Sugar, etc), kg/kg P
α_{381}	Others (Alcoholic beverages, Veg. Oil, Sugar, etc), kg/kg C
α_{382}	Others (Alcoholic beverages, Veg. Oil, Sugar, etc), Kcal/kg E
α_{383}	CORN FOR SILAGE, kg/kg N
α_{384}	CORN FOR SILAGE, kg/kg P
α_{385}	CORN FOR SILAGE, kg/kg C
α_{386}	CORN FOR SILAGE, Kcal/kg E
α_{387}	ALL HAY INCLUDING ALFALFA , kg/kg N
α_{388}	ALL HAY INCLUDING ALFALFA , kg/kg P
α_{389}	ALL HAY INCLUDING ALFALFA , kg/kg C
α_{390}	ALL HAY INCLUDING ALFALFA , Kcal/kg E
α_{391}	Initial Soil Nutrient Content: Grass and lawn, kg/ha N
α_{392}	Initial Soil Nutrient Content: Grass and lawn, kg/ha P
α_{393}	Initial Soil Nutrient Content: Grass and lawn, kg/ha C
α_{394}	Initial Soil Nutrient Content: Grass and lawn, - E
α_{395}	Initial Soil Nutrient Content: Forests, kg/ha N
α_{396}	Initial Soil Nutrient Content: Forests, kg/ha P
α_{397}	Initial Soil Nutrient Content: Forests, kg/ha C
α_{398}	Initial Soil Nutrient Content: Forests, - E
α_{399}	Initial Soil Nutrient Content: Crops and Pasture, kg/ha N
α_{400}	Initial Soil Nutrient Content: Crops and Pasture, kg/ha P
α_{401}	Initial Soil Nutrient Content: Crops and Pasture, kg/ha C
α_{402}	Initial Soil Nutrient Content: Crops and Pasture, - E
α_{403}	Live Animal - Cattle, kg/kg N

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Continued from previous page

ID	Description
α_{404}	Live Animal - Cattle, kg/kg P
α_{405}	Live Animal - Cattle, kg/kg C
α_{406}	Live Animal - Cattle, Kcal/kg E
α_{407}	Live Animal - Poultry, kg/kg N
α_{408}	Live Animal - Poultry, kg/kg P
α_{409}	Live Animal - Poultry, kg/kg C
α_{410}	Live Animal - Poultry, Kcal/kg E
α_{411}	Live Animal - Pig, kg/kg N
α_{412}	Live Animal - Pig, kg/kg P
α_{413}	Live Animal - Pig, kg/kg C
α_{414}	Live Animal - Pig, Kcal/kg E
α_{415}	Cattle Feed Requirements, % DM Protein
α_{416}	Cattle Feed Requirements, % DM Fat
α_{417}	Cattle Feed Requirements, % DM carbohydrates
α_{418}	Cattle Feed Requirements, % DM P
α_{419}	Cattle Feed Requirements, Kcal/kg E
α_{420}	Poultry Feed Requirements, % DM Protein
α_{421}	Poultry Feed Requirements, % DM Fat
α_{422}	Poultry Feed Requirements, % DM carbohydrates
α_{423}	Poultry Feed Requirements, % DM P
α_{424}	Poultry Feed Requirements, Kcal/kg E
α_{425}	Pig Feed Requirements, % DM Protein
α_{426}	Pig Feed Requirements, % DM Fat
α_{427}	Pig Feed Requirements, % DM carbohydrates
α_{428}	Pig Feed Requirements, % DM P
α_{429}	Pig Feed Requirements, Kcal/kg E
α_{430}	EGG composition (as w/w of edible portion of egg), % Protein
α_{431}	EGG composition (as w/w of edible portion of egg), % Fat
α_{432}	EGG composition (as w/w of edible portion of egg), % carbohydrates
α_{433}	EGG composition (as w/w of edible portion of egg), % P
α_{434}	EGG composition (as w/w of edible portion of egg), Kcal/kg E
α_{435}	Milk composition, % Protein
α_{436}	Milk composition, % Fat
α_{437}	Milk composition, % carbohydrates
α_{438}	Milk composition, % P
α_{439}	Milk composition, Kcal/kg E
α_{440}	,
α_{441}	,
α_{442}	,
α_{443}	,
α_{444}	Natural gas (NG) composition - dry basis, % w/w N
α_{445}	Natural gas (NG) composition - dry basis, % w/w P

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Continued from previous page

ID	Description
α_{446}	Natural gas (NG) composition - dry basis, % w/w C
α_{447}	Natural gas (NG) composition - dry basis, kWh/std m3 E
α_{448}	,
α_{449}	,
α_{450}	,
α_{451}	,
α_{452}	Coal composition, % w/w N
α_{453}	Coal composition , % w/w P
α_{454}	Coal composition, % w/w C
α_{455}	Coal composition, kWh/tonne E
α_{456}	Diesel composition, % w/w N
α_{457}	Diesel composition, % w/w P
α_{458}	Diesel composition, % w/w C
α_{459}	Diesel composition, kWh/tonne E
α_{460}	Gasoline composition, % w/w N
α_{461}	Gasoline composition, % w/w P
α_{462}	Gasoline composition, % w/w C
α_{463}	Gasoline composition, kWh/tonne E
α_{464}	Composition fuel Alternative f1, % w/w N
α_{465}	Composition fuel Alternative f2, % w/w P
α_{466}	Composition fuel Alternative f3, % w/w C
α_{467}	Composition fuel Alternative f4, kWh/tonne E
α_{468}	Composition fuel Alternative f1, % w/w N
α_{469}	Composition fuel Alternative f2, % w/w P
α_{470}	Composition fuel Alternative f3, % w/w C
α_{471}	Composition fuel Alternative f4, kWh/tonne E
α_{472}	Composition fuel Alternative f3, % w/w N
α_{473}	Composition fuel Alternative f4, % w/w P
α_{474}	Composition fuel Alternative f5, % w/w C
α_{475}	Composition fuel Alternative f6, kWh/tonne E
α_{476}	O horizon layer in UNDISTURBED forests, g/m2 N
α_{477}	O horizon layer in UNDISTURBED forests, g/m2 P
α_{478}	O horizon layer in UNDISTURBED forests, g/m2 C
α_{479}	O horizon layer in UNDISTURBED forests, - E
α_{480}	,
α_{481}	,
α_{482}	,
α_{483}	,
α_{484}	,
α_{485}	,
α_{486}	,
α_{487}	,

Continued on next page

Continued from previous page

ID	Description
α_{488}	,
α_{489}	,
α_{490}	,
α_{491}	,
α_{492}	,
α_{493}	,
α_{494}	,
α_{495}	,
α_{496}	Nutrient content in WET deposition, mg/L N
α_{497}	Nutrient content in WET deposition, mg/L P
α_{498}	Nutrient content in WET deposition, mg/L C
α_{499}	Nutrient content in WET deposition, E
α_{500}	Nutrient content in DRY deposition, kg/ha.y N
α_{501}	Nutrient content in DRY deposition, kg/ha.y P
α_{502}	Nutrient content in DRY deposition, kg/ha.y C
α_{503}	Nutrient content in DRY deposition, E
α_{504}	Total Population (first year of simulation), cap x 103
α_{505}	Maximum population in the study area for t -¿ ?, cap x 103
α_{506}	Total Area (not changing in time), km2
α_{507}	Impervious area, percentage
α_{508}	Water consumption for Mining, Mgal/d
α_{509}	Inventory of Cattle and Calves, heads x 103
α_{510}	Inventory of Poultry, heads x 103
α_{511}	Inventory of hogs and pigs , heads x 103
α_{512}	Fraction of Forested Areas, ratio
α_{513}	Fraction of low intensity urban areas, ratio
α_{514}	Fraction of high intensity urban areas, ratio
α_{515}	Fraction of crop and pastures, ratio
α_{516}	Fraction of open water and wetland areas, ratio
α_{517}	Recreational areas subject to irrigation (first year), km2
α_{518}	capacity for power generation - Coal , MW
α_{519}	capacity for power generation - NG, MW
α_{520}	capacity for power generation - Nuclear, MW
α_{521}	capacity for power generation - Diesel, MW
α_{522}	capacity for power generation - Hydro, MW
α_{523}	capacity for power generation - Alternative p1, MW
α_{524}	capacity for power generation - Alternative p2, MW
α_{525}	capacity for power generation - Alternative p3, MW
α_{526}	capacity for fuel production - Alternative f1, Mgal/d
α_{527}	capacity for fuel production - Alternative f2, Mgal/d
α_{528}	capacity for fuel production - Alternative f3, Mgal/d
α_{529}	Previous year precipitation (year = 0), mm

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ID	Description
α_{530}	Long term average Precipitation, mm
α_{531}	Long term minimum precipitation, mm
α_{532}	Long term maximum precipitation, mm
α_{533}	Atmospheric vapor pressure, mbar
α_{534}	Average Air temperature, C
α_{535}	Average Wind Velocity, km/day
α_{536}	Average latitude of the system, degrees
α_{537}	Surface water reservoir initial elevation, m-msl
α_{538}	Fraction of forest areas as timberland, ratio
α_{539}	Softwood - Live trees volume, m3 x 103
α_{540}	Hardwood - Live trees volume, m3 x 103
α_{541}	Sawmills total capacity, bf x 106
α_{542}	Average Cattle weight , kg/head
α_{543}	Average Poultry Weight, kg/head
α_{544}	Average Pig weight, kg/head
α_{545}	Fraction of Cows for Milk , ratio
α_{546}	Fraction of layers, ratio
α_{547}	Milk yield per cow, kg/head.y
α_{548}	Egg yield per layer hen, eggs/head.y
α_{549}	Number of people per household, cap/house
α_{550}	Natural Gas density (60 F), kg/m3
α_{551}	Diesel density (60 F), kg/m3
α_{552}	Gasonlines density (60 F), kg/m3
α_{553}	capacity for power generation - Geothermal, MW
α_{554}	capacity for power generation - Wind, MW
α_{555}	Average Car fuel mileage, km/L
α_{556}	Average human weight, kg
α_{557}	Precipitation (mm), mm
α_{558}	Surface Drainage Mgal/d, Mgal/d
α_{559}	End-of-year reservoir level m-msl, m-msl
α_{560}	IBT of water Mgal/d (a), Mgal/d
α_{561}	IBT of wastewater Mgal/d (a), Mgal/d
α_{562}	Cap increase PG - Coal MW, MW
α_{563}	Cap increase PG - NG MW, MW
α_{564}	Cap increase PG - Nuclear MW , MW
α_{565}	Cap increase PG - Diesel MW , MW
α_{566}	Cap increase PG - MW p1 , MW
α_{567}	Cap increase PG - MW p2, MW
α_{568}	Cap increase PG - MW p3, MW
α_{569}	Cap increase FP - MW Alt f1 , MW
α_{570}	Cap increase FP - MW Alt f2, MW
α_{571}	Cap increase FP - MW Alt f3, MW

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ID	Description
α_{572}	Cap increase sawmill, M bf
α_{573}	Cap increase PG - Geo MW, MW
α_{574}	Cap increase PG - Wind MW, MW

Appendix C

Model Code Structure

The code of the Multi-sectoral Systems Analysis (MSA) framework is developed in MATLAB® with a structure that resembles the division of industrial sectors, i.e. water, forestry, food, energy, and waste management. As shown in Figure C.1, the model is comprised of four parts. The first part involves reading the input file, *MSSAinput.xls*, which contains several worksheets that organize the input information into: (i) model running options, (ii) parameters and inputs. Data are organized into matrices by the 'dataready' module. The second block contains the Regionalized Sensitivity Analysis (RSA) code, which is similar to the one presented by Osidele (2001). In this part, the model decides whether to execute the MSA together with the RSA procedure or not, based on the options selected by the analyst. The core of the MSA code, the third part, is divided into eight modules that include:

1. 'prelim': realizes preliminary calculations such as population and land use distribution.
2. 'waters': performs calculations related to hydrologic processes, consumption of water resources, wastewater treatment, and discharges to aquatic systems. It also estimates the production of domestic wastewater and the energy content of those flows which are predominantly water.
3. 'forestrys': estimates wood production, yard waste generation, atmospheric deposition of nutrients, and nutrient applied to land. With the latter, the model is able to estimate the nutrient content in those flows associated with runoff and soil infiltration flows.

4. ‘foods’: calculates the flows associated the consumption and production of livestock, fodder, and food.

5. ‘wastems’: includes the different technologies utilized to process, treat, or dispose wastes that are generated in the water, forestry, food, and energy sectors. Some of the processes are incineration, landfilling, composting, and the two alternative technologies: pyrolysis and struvite production. The energy generated in this sector is also estimated.

6. ‘energys2’: carries out the calculations associated with the energy sector by estimating the energy requirements of the system and the emissions released from power generation and fuels use.

7. ‘out_main’: calculates the emissions of the *reference* state, classifies flows, and determines the value of the indicators.

8. ‘Export’: prepares and formats the generated information before transferring it to the output file.

The last, and fourth block, corresponds to the generation of the output tables, which are created in an output file, *MSSAout.xls*. These tables include the various flows for each species, sustainability indicators, RSA results, and the aggregated flows, i.e. products, resources, waste, air emissions, and aquatic emissions.

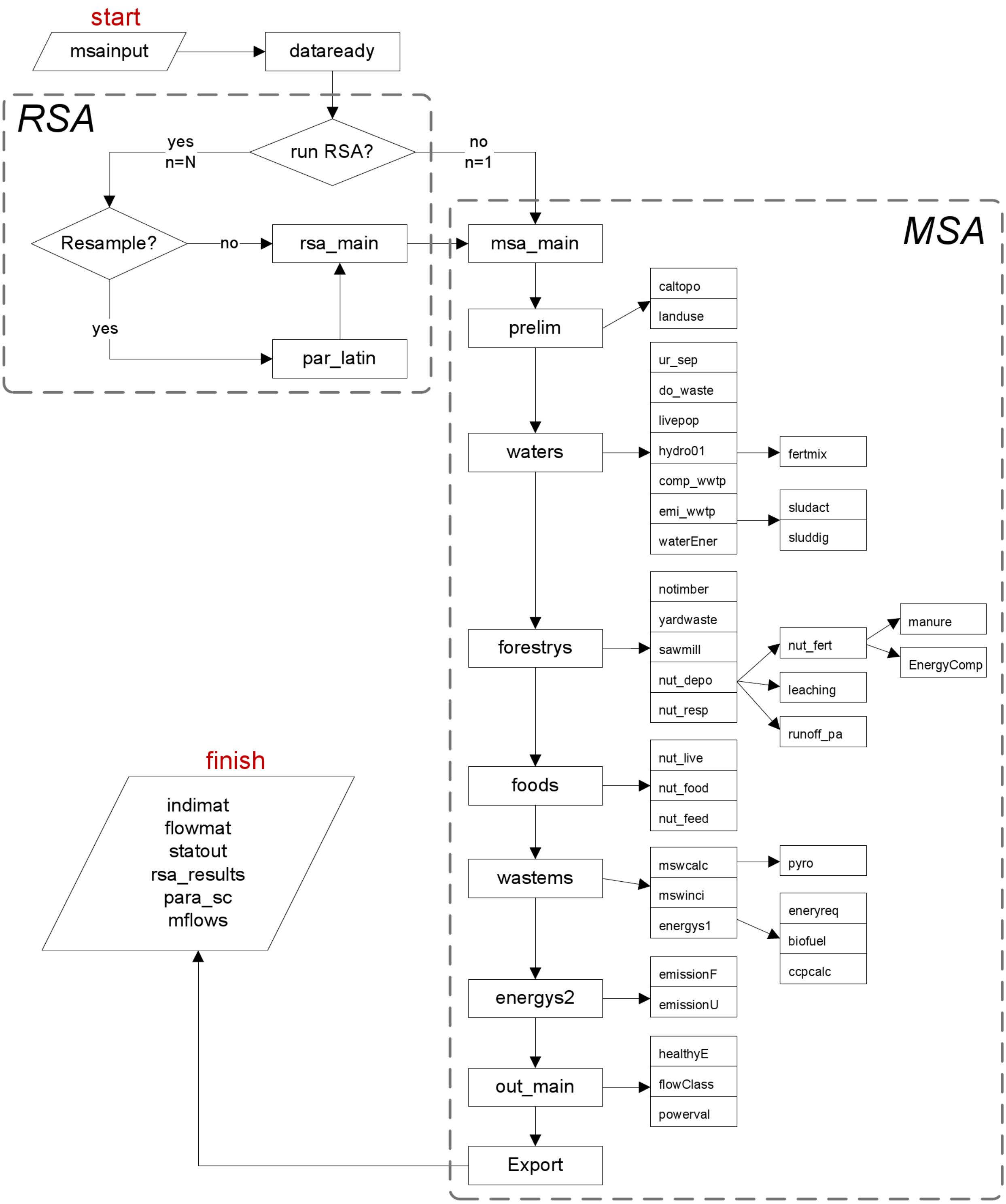

Figure C.1: Structure of the model code for the Multi-sectoral Systems Analysis and Regionalized Sensitivity Analysis.

Appendix D

Material Flow Diagrams for Nitrogen

The present Appendix includes the flow diagrams introduced in Chapter 3, but this time as a vehicle to show, in a visual manner, the inputs, outputs, and internal mass flows of nitrogen across the five sectors. The same practice can be done with water, phosphorus, carbon, and energy. as an example.

Figures D.1, D.2, D.3, D.4, and D.5 show the mass of nitrogen corresponding to the *base case* (for the year 2000) in the water, forestry, food, energy, and waste management sectors respectively.

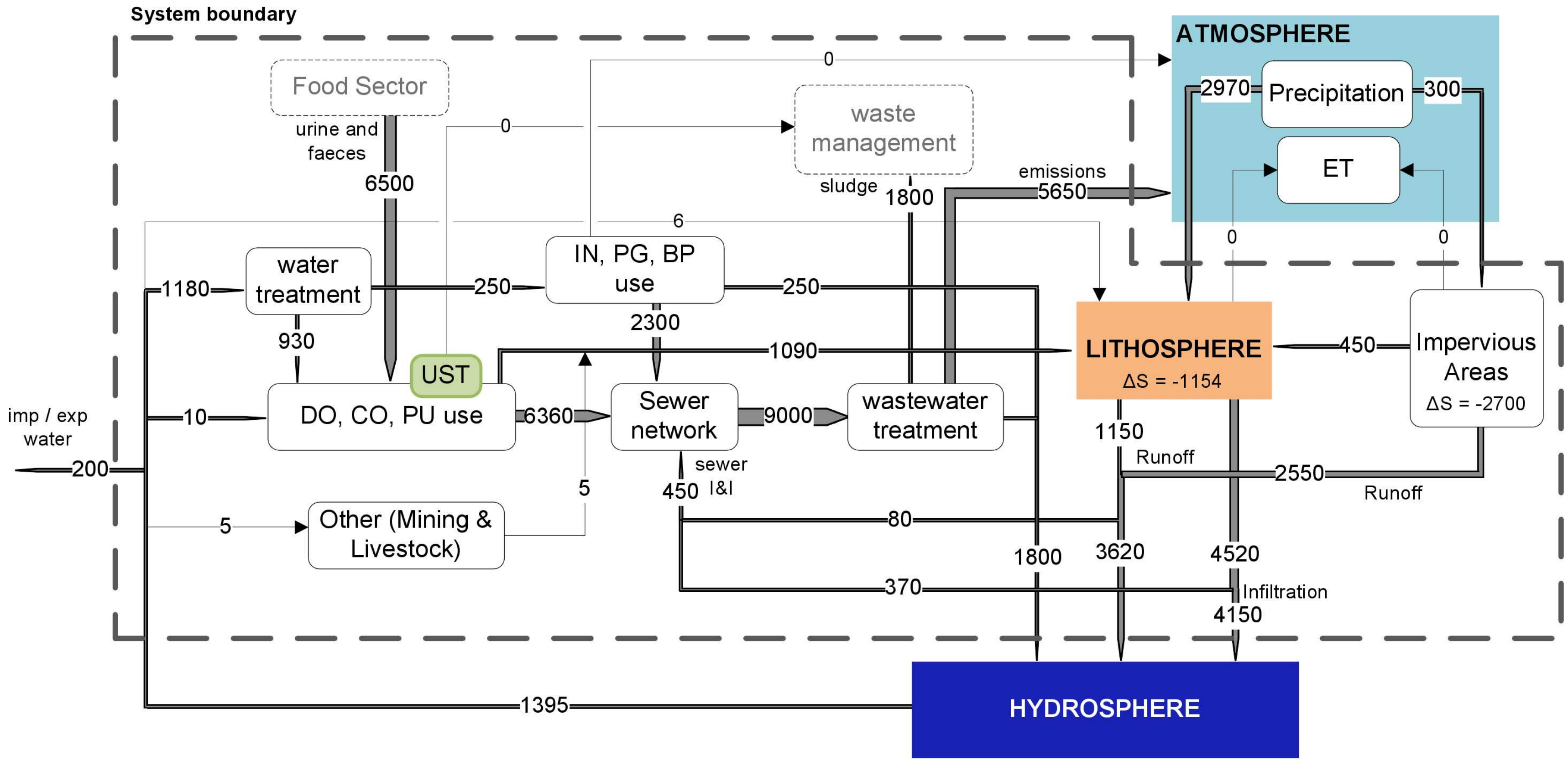

Figure D.1: Material flow diagram of nitrogen through the water sector. All flows and accumulation rates reported as $\mathrm{t\,N\,y^{-1}}$. Abbreviations: DO domestic or residential; CO commercial; PU public; PG power generation; BP biofuel production; IN industrial; ET evapotranspiration; PA pervious areas; IA impervious areas; UST urine separation technology (not active for the *base case*; ΔS is the accumulation rate in $\mathrm{t\,N\,y^{-1}}$.

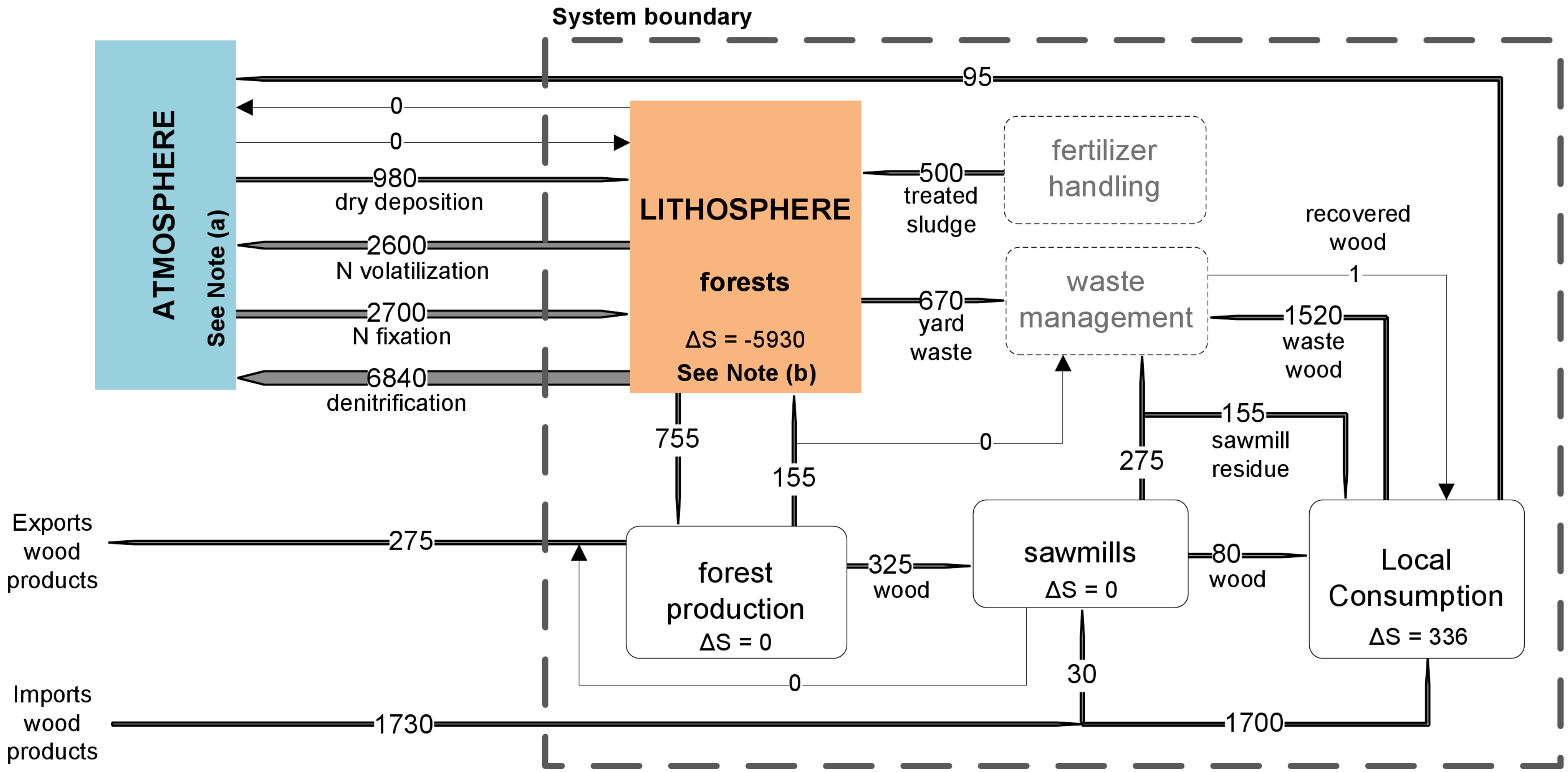

Figure D.2: Material flow diagram of nitrogen through the forestry sector. All flows and accumulation rates reported as $\mathrm{t\,N\,y^{-1}}$. Abbreviations: ΔS is the accumulation rate in $\mathrm{t\,N\,y^{-1}}$.
Note (a): Flows between the lithosphere and the atmosphere, such as plant respiration and photosysthesis, N volatilization, denitrification, deposition, and N fixation include those flows corresponding to the food sector (see Figure D.3).
Note (b): The accumulation of N has to be considered together with the accumulation of the food sector (see Figure D.3).

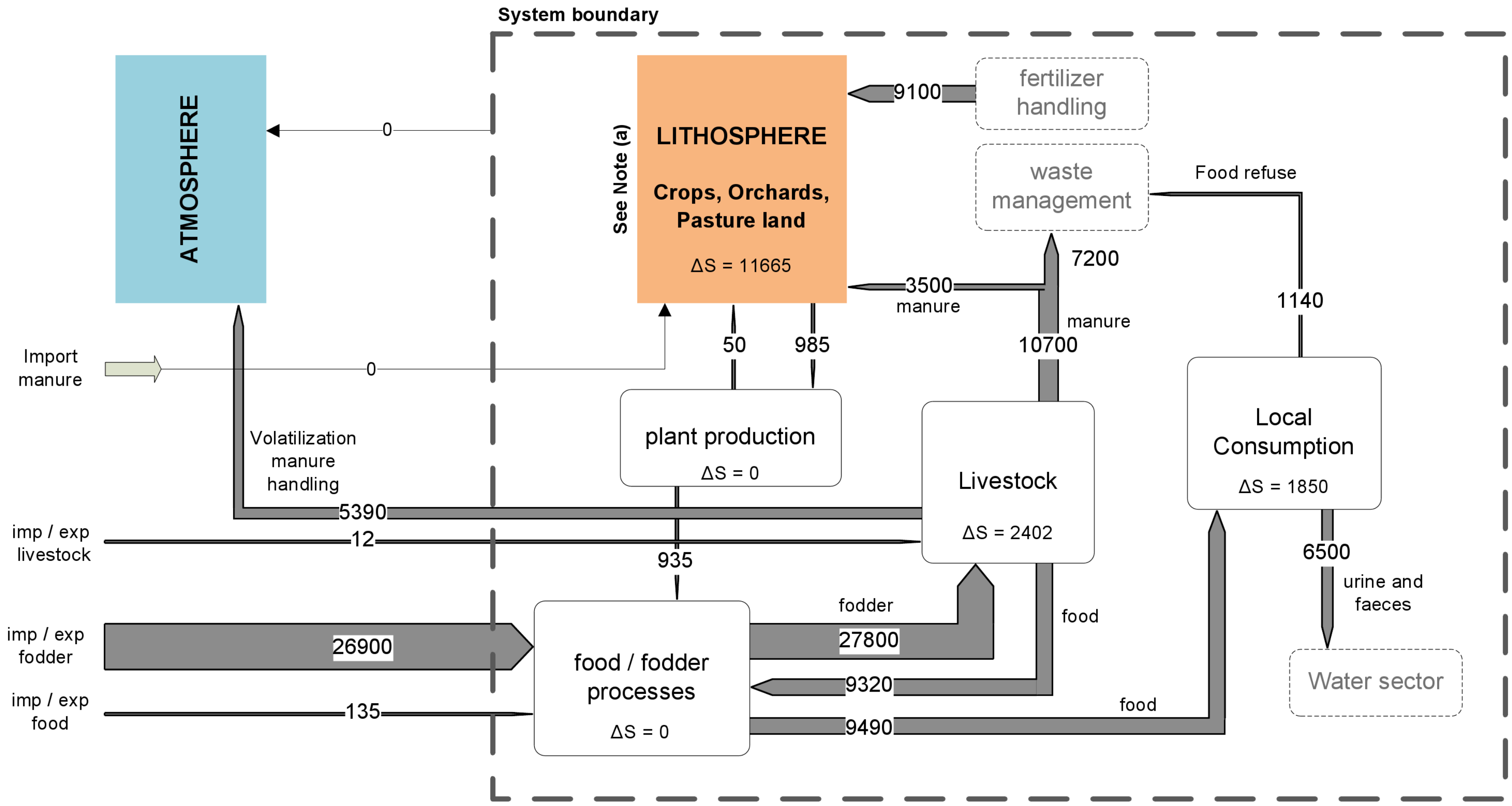

Figure D.3: Material flow diagram of nitrogen through the food sector. All flows and accumulation rates reported as $\mathrm{t\,N\,y^{-1}}$. Abbreviations: ΔS is the accumulation rate in $\mathrm{t\,N\,y^{-1}}$.
Note (a): Flows between the lithosphere and the atmosphere such as plant respiration and photosysthesis, N volatilization, denitrification, deposition, and N fixation are all aggregated as part of the forestry sector in Figure D.2.

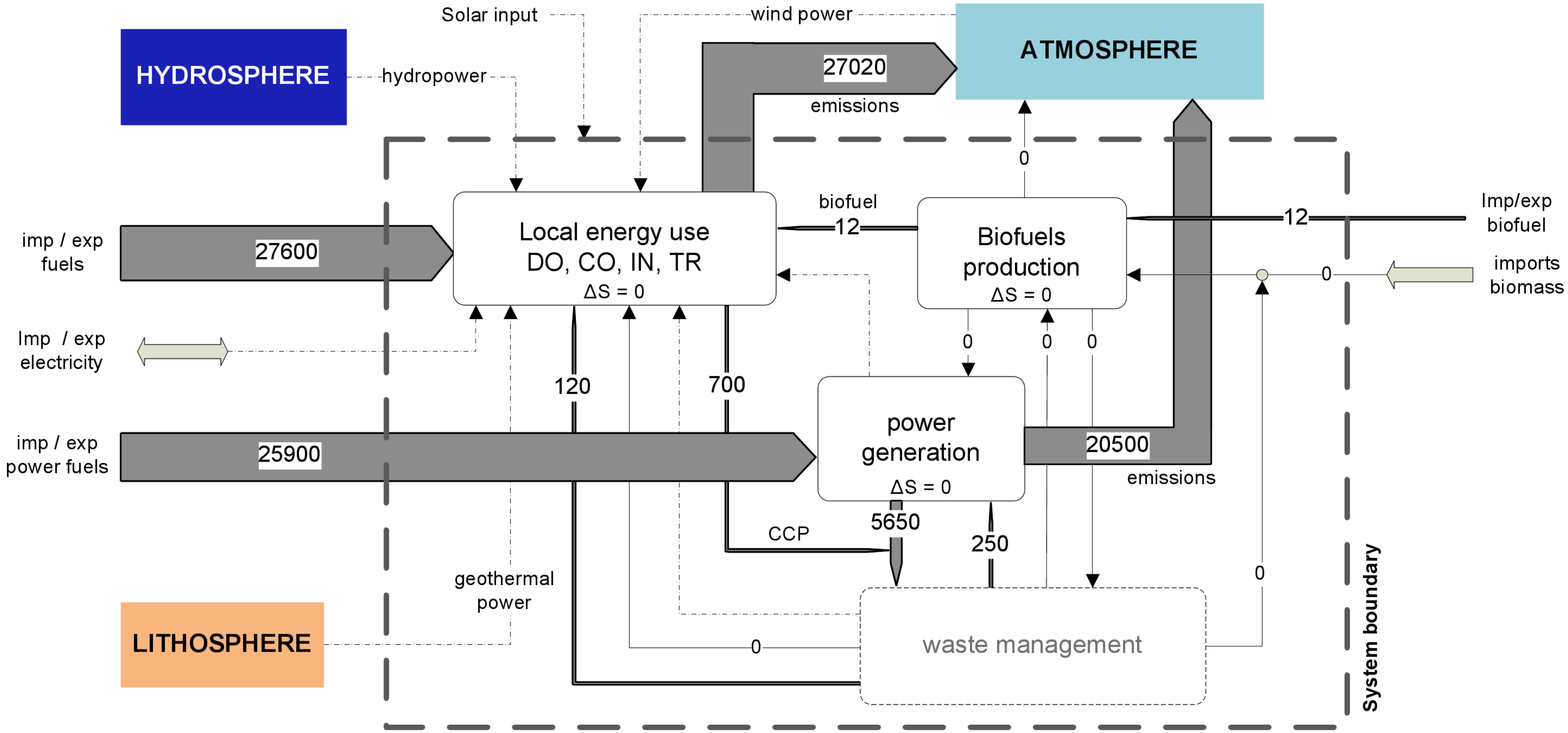

Figure D.4: Material flow diagram of nitrogen through the energy sector. All flows and accumulation rates reported as $\mathrm{t\,N\,y^{-1}}$. Abbreviations: DO domestic or residential; CO commercial; IN industrial; TR transportation; CCP: Coal Combustion Products; ΔS is the accumulation rate in $\mathrm{t\,N\,y^{-1}}$.

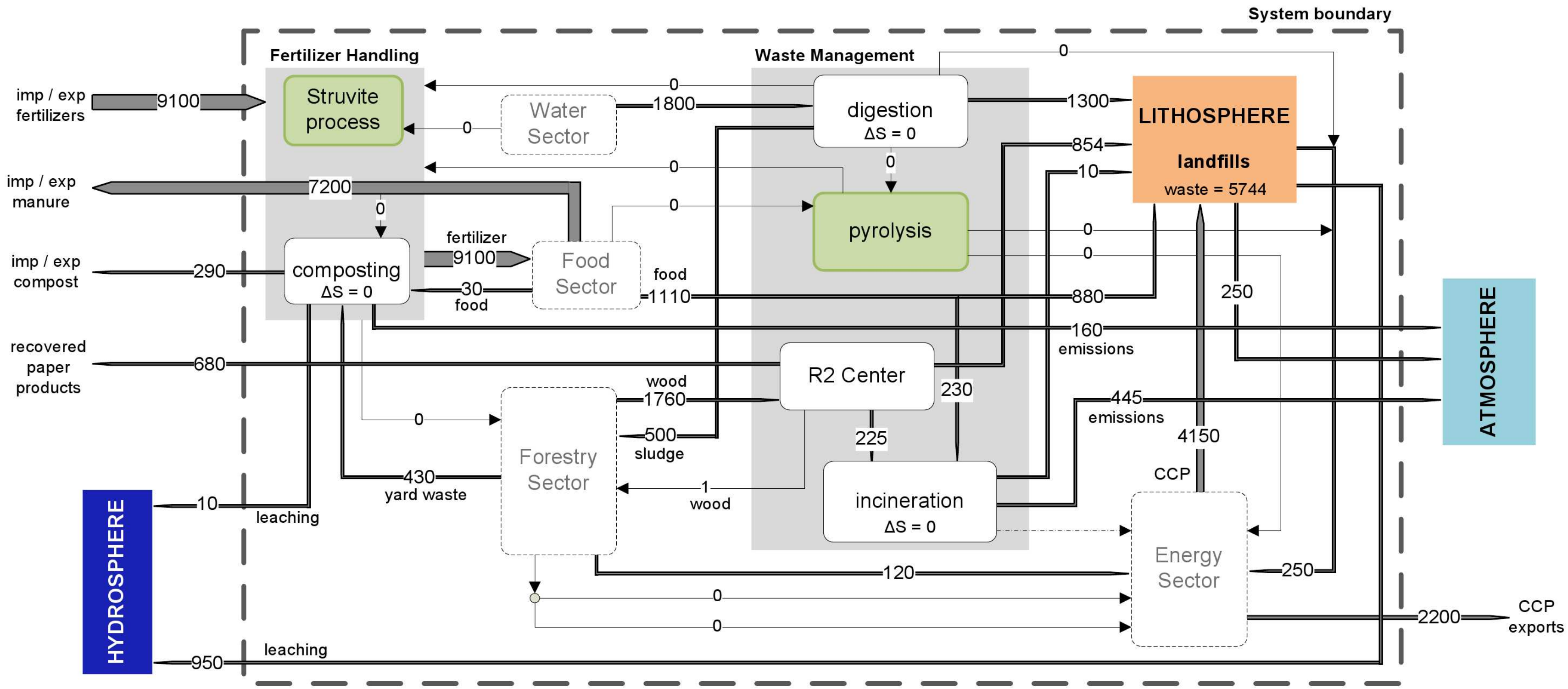

Figure D.5: Material flow diagram of nitrogen through the waste management sector. All flows and accumulation rates reported as $\mathrm{t\,N\,y^{-1}}$. Abbreviations definitions: R2 recycling and reusing; CCP coal combustion products; ΔS is the accumulation rate in $\mathrm{t\,N\,y^{-1}}$.

Appendix E

Mathematical Behavior of Indicators

The behavior, i.e., the solution space, of the four indicators related to efficiency and eco-efficiency (indicators PRI, RWI, PWI, and EEI) can be considered straightforward and easier to understand than those indicators that use the reference state as part of their mathematical structure. Therefore, the following explanation is devoted to the latter group, comprised of indicators HWE, HAE, WEF, and E2I. Although E2I is not explicitly described, it is possible to explain its behavior by understanding indicators HWE, HAE, and WEF, because the eco-effective indicator (E2I) is basically an aggregation of these three indicators.

With regard to the indicator HAE (healthy atmospheric emissions), both numerator, E_k^0, and denominator, E_k, can change in sign (positive or negative); therefore, the behavior of HAE is described in two figures: Figure E.1 for $\mathrm{E}_k^0 > 0$, and Figure E.2 when $\mathrm{E}_k^0 < 0$. As shown in these two figures, when E_k approaches zero, the value of the indicator tends to $-\infty$ or $+\infty$. Based on the curves, it is also observed that when the value of HAE moves towards $-\infty$ it represents an improvement of the system's performance. Indicator WEF (waste equals food), in Figure E.4, can be interpreted similarly to HAE when $\mathrm{E}_k^0 > 0$.

On the other hand, HWE (healthy water emissions) is always a positive value, since aquatic emissions are considered to be exiting from the system in all cases, i.e., A_k^0 and A_k are always < 0. Thus, its behavior is expected to be similar to that of indicators PRI, RWI, PWI, and EEI, as shown in Figure E.3.

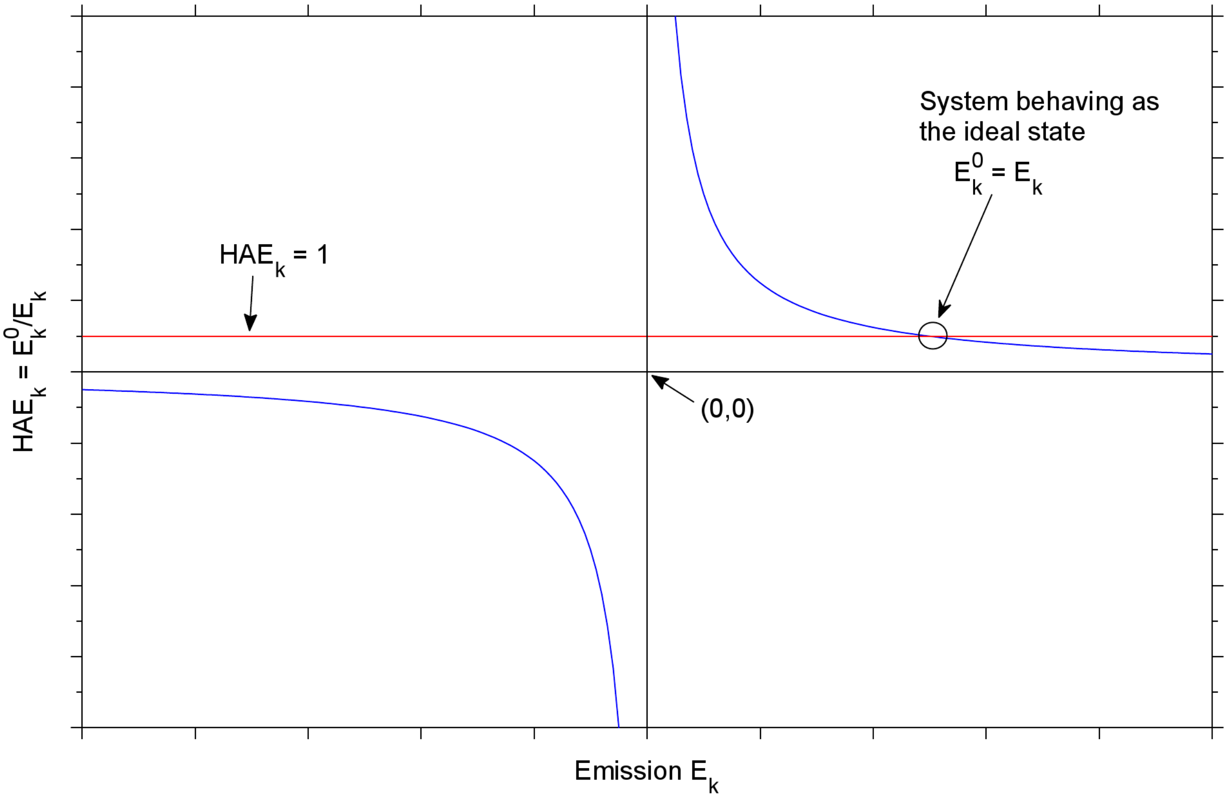

Figure E.1: Solution space of indicator HAE for a $E_k^0 > 0$.

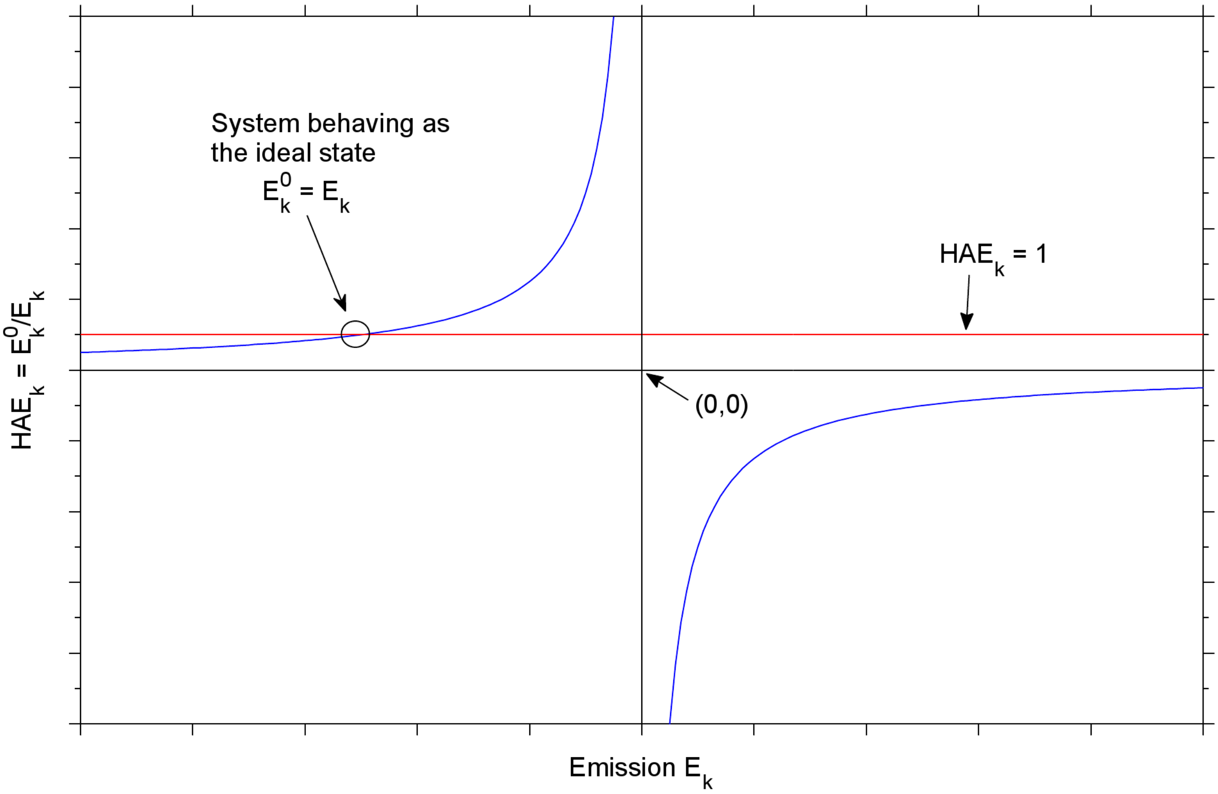

Figure E.2: Solution space of indicator HAE for a $E_k^0 < 0$.

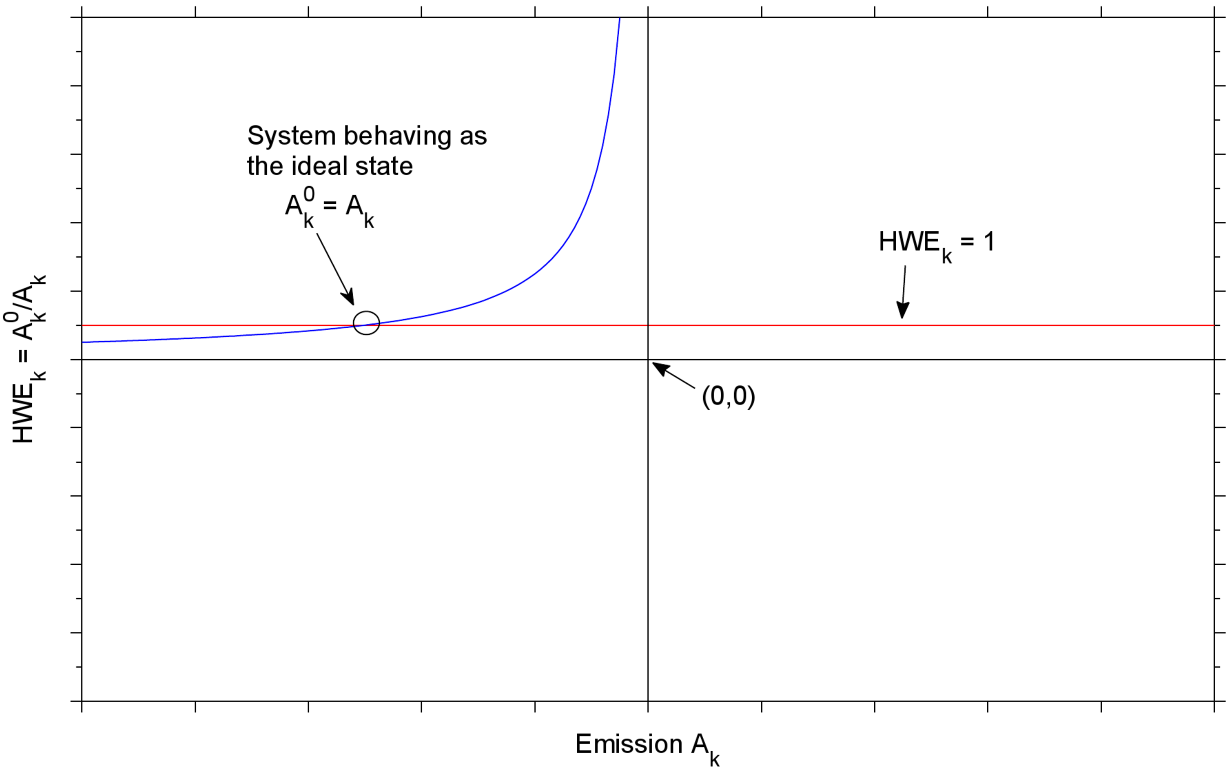

Figure E.3: Solution space of indicator HWE. A_k^0 and A_k always < 0.

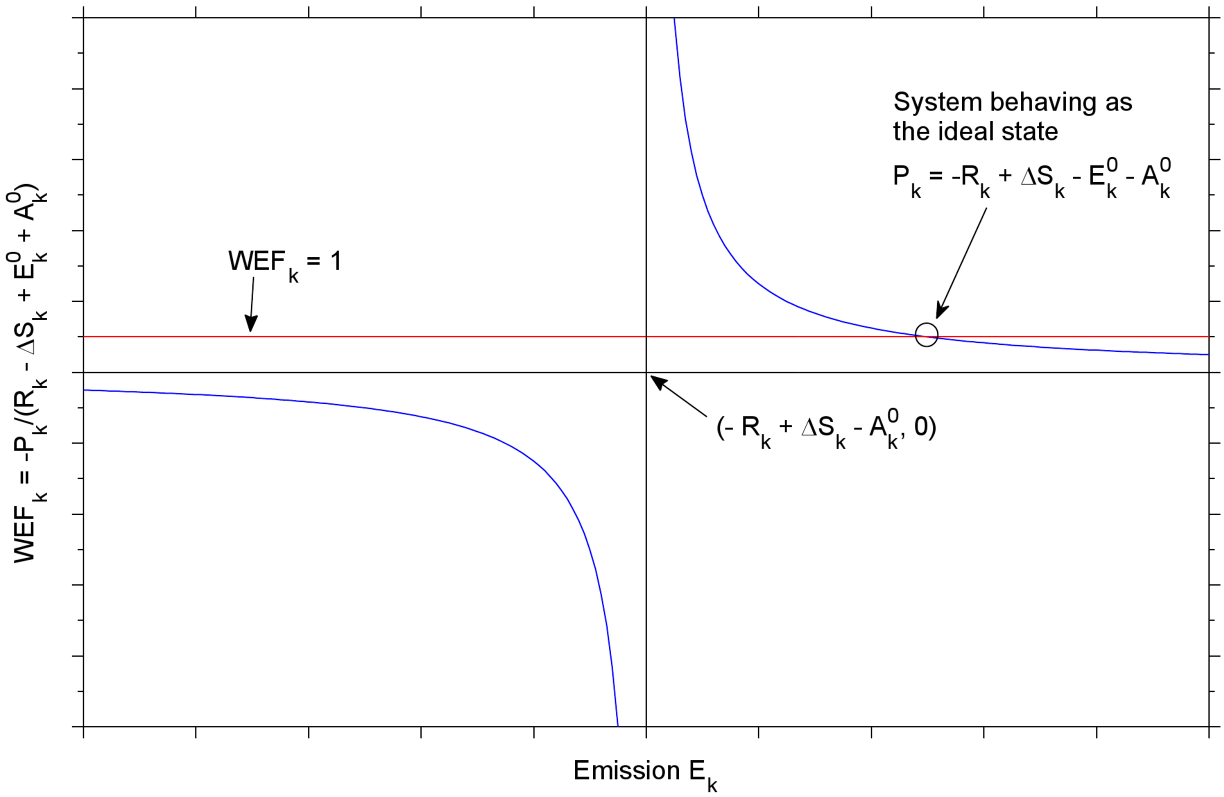

Figure E.4: Solution space of indicator WEF.