PLANTS IN THE GARDEN: AN APPROACH TO MODELING THE IMPACT OF
INDUSTRIAL ACTIVITIES IN ECOSYSTEMS

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Plants in the Garden: An Approach to Modeling the Impact of
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NOMENCLATURE

Anthropogenic – Created or caused by mankind

Anthro-Ecosphere – The union of the anthrosphere and ecosphere; the union of the things of mankind and those of non-sentient living world

Deposited Organic Material (DOM) – organic material remaining in a cell after the death and decomposition of biomass (Voinov, et al. 2002)

Geographical Information Systems (GIS) – Software systems used to archive and manipulate geographical and related types of data

Manning Coefficient – A parameter representing the resistance to surface fluid flow caused by vegetation

Matlab – Software used for technical computing

M2 – A software map format particular to Apple operating systems

Net Primary Production or Total Net Primary Productivity (NPP) – the total amount of biomass added to a plant or group of plants during an observed period of time

Net Primary Productivity – "…the rate of storage of organic matter in plant tissues exceeding the respiratory use…" (Odum 1987)

Non-photosynthetic Biomass – living plant tissue that provides functions other than photosynthesis (ex. tree trunk)

Photosynthetic Biomass – living plant tissue that is capable of photosynthesis (ex. leaves)

Patuxent Landscape Model (PLM) – a spatially explicit, dynamic ecosystem landscape model of the Patuxent River watershed in Maryland (Costanza, et al. 2002)

Portable Pix Maps (PPM) – A basic data format usually used for images

Saturated Water – water stored in a subsurface soil zone where all of the pore space is occupied by water (Voinov, et al. 2002)

Surface Water – water temporarily stored above ground as runoff or part of a body of water such as a pond, lake, creek or river

Spatial Modeling Environment (SME) – software used to unite and transform individual ecosystem process modules into spatially explicit, dynamic ecosystem landscape models

Triple Bottom Line (TBL) – a corporate performance measurement standard within the context of sustainable development that implicitly sets the "…simultaneous pursuit of economic prosperity, environmental quality and social equity…" as goals for every company (Elkington 1998)

Unconfined Aquifer – "…a body of saturated sediment or rock that is not directly overlain…" by impermeable or nearly impermeable material (Hudak 1999)

Unsaturated Water – water stored in a subsurface soil zone where pore space is occupied by water and air or other gases (Voinov, et al. 2002). This layer usually sits atop the saturated layer.

SUMMARY

Humanity's interactions with the supporting environment are, to state the obvious, complex. Humanity's industrial activities effect the environment over time and space, and the same activities even produce different results in different locations. Since the complexities of these interactions may preclude the successful use of eco-performance metrics, humanity may need a means of informing environmental management decisions that accounts for changes with time, spatial patterns and local uniqueness. The objective of this effort is to interface engineering and ecological systems models to better estimate environmental impacts by modeling the dynamic, spatially explicit and location dependent changes caused by industrial activities. Building upon previously developed, dynamic, spatially explicit, location specific ecosystem modeling software, a technical framework for estimating the impacts of industrial systems in ecosystems is developed. Ecological disturbances endemic to engineering systems are integrated into these existing ecosystem models. The results of these integrations are discussed, and from these results, the potential for estimating impacts using dynamic, spatially explicit and location based modeling is evaluated. In other words, one learns the result of placing industrial plants in mother nature's garden.

CHAPTER 1

Motivation, Goals and Questions

1.1 Overarching Motivation

We choose to go to the moon in this decade and do the other things, not because they are easy, but because they are hard, because that goal will serve to organize and measure the best of our energies and skills, because that challenge is one that we are willing to accept, one we are unwilling to postpone, and one which we intend to win…

John F. Kennedy, 1962

What is sustainability? What are the differences between sustainable and unsustainable activities? How can mankind achieve the former and avoid the dire consequences of the later? Short of waiting until the end of days, how will a society, region or locale know when it has achieved sustainability? These four questions comprise the core of the sustainability debate. From the coasts of Spain and Portugal blackened by the 2002 Prestige oil spill to the smog filled skies of Atlanta, one cannot help but notice the burden mankind places upon the thin biological shell encapsulating this rock orb called Earth. And, the obnoxious output at the pipe's end often distracts attention from the ever-growing maw that is the pipe's mouth. Wedged between waste assimilation and consumption, the pressure on the biosphere increases with each

additional member of the human race, and mankind's need to answer the four previously mentioned questions becomes more acute.

In response to the global need for answers, politicians, philosophers, scientists and others proposed and continue to propose definitions for sustainability, and based on these definitions, they divine the difference between sustainable and unsustainable actions. Scientists, technologists and entrepreneurs tackle the problem of how to implement visions of sustainability while striving to avoid the all too unsustainable present realities. These efforts produce definitions, interpretations of definitions, lists of requirements, schemes, methods and technological artifacts for sustainability. Undoubtedly, the fruits of these labors will prove savory.

But in the din about direction and movement, destination is being lost; the fourth question, the child's question, "are we there yet?," is receiving short shrift. Technologies and management methods meant to alleviate the pressure on the biosphere while sustaining economic activity come into existence, but mankind lacks the means of discerning whether these developments result in a more sustainable enterprise or society. At its heart, this work is a response to the fourth question. In a technical and detailed, though limited way, this work begins the process of answering the question, 'how will a society, region or locale know when it has achieved sustainability?' And in a fashion similar to the moon landing, this and other sustainability endeavors hopefully, "will serve to organize and measure the best of our energies and skills," but unlike the moon shot, all must understand that humanity cannot decline this challenge.

1.2 Scope

Since defining, progressing toward, achieving and maintaining a sustainable society is a grand human endeavor, one work cannot hope to contain the entire solution. Furthermore, the process of verifying actions and conditions as sustainable encompasses far more than the contents of one thesis. Therefore, this work focuses upon a portion of two of the three primary elements of sustainability (i.e. environmental, economic and social sustainability). Beginning to understand the sustainability of industrial and ecological activities at the local and regional levels is within the scope of a thesis; so, it is upon these portions of sustainability's economic and environmental pillars that this work focuses. The specific goal of this research follows.

My **goal** is to specify and develop the fundamental building blocks of a technical framework for integrating local and regional industrial and ecological models that, when united, estimate the environmental impact of industrial decisions and begin to assess the sustainability of actions and patterns of actions.

1.2.1 Sustainability – Context and Relevance

Section 1.1 commences with questions involving a deceptively simple word – sustainability. Most possess a partial, intuitive understanding of what sustainability means, but as previously mentioned, this work focuses upon only a portion of the subject-matter encompassed by sustainability. To align a reader's understanding of sustainability with the one used in this thesis, one must define sustainability. And, to demonstrate this

work's relevance to sustainability, one must select and discuss elements of definitions which correspond to the presented goal.

Many definitions for sustainability exist, and most overlap to some degree. The following list of definitions provides a representative sample.

1. "Meeting the needs of the present generation without compromising the ability of future generations to meet their needs." – Brundtland, 1987

2. Sustainable – capable of being sustained or maintained; maintainable (Webster's New Universal Unabridged Dictionary Deluxe 2nd Edition 1972)

3. Sustain - to maintain; to keep in existence; keep going; prolong; to keep supplied with necessities; to suffer; to endure (Webster's New Universal Unabridged Dictionary Deluxe 2nd Edition 1972)

4. "A thing is right when it tends to preserve the integrity, stability and beauty of the biotic community. It is wrong when it tends otherwise" (Leopold 1948).

5. "…a sustainable system is one which survives or persists…" (Costanza, et al. 1997)

6. "Sustainability…is a general obligation to preserve the capacity to be well off, to be as well off as we" (Solow 1991).

As one may note, the more vague the definition the more acceptable it appears. As one contemplates the underlying meaning of the more concrete definitions (4 and 6), certainty begins to erode. Is the entire biotic community more important than the human sub-community, and exactly what or who must remain "well off"?

This collection of definitions does reveal two important facts. First, different thinkers propose and defend different perspectives. Second, the context surrounding these definitions reveals that sustainability consists of *environmental, economic and social* components, though not all authors recognize all three components (Solow 1991). These three components of sustainability are the reason for the much discussed triple bottom line – the environmental, economic and social values that a company focusing on sustainability would seek to increase.

Despite ambiguities and uncertainties, definitions four, five and six provide the necessary context for sustainability because they respectively focus on the environmental and economic pillars. They situate this work within the realm of the environmental and economic bottom lines. The fourth definition centers on the need to sustain the biotic community. The goal statement's attention to ecological modeling connects this work with the fourth definition. The sixth definition centers on the preservation of "the capacity to be well off." Part of this capacity is industrial; so, the goal's focus on industrial modeling connects it to the sixth definition. And, general attention to sustainable decisions connects the goal with the fifth definition. Connections between the listed sustainability definitions and the goal statement provide the foundation for a working definition of sustainability.

> Sustainability (a working definition) – a persistent state of a coupled ecological and economic system that preserves biotic integrity and stability while simultaneously allowing human inhabitants "to be well off."

With the bounds of this work circumscribed by sustainability definitions and with the relevance of this work established by connections to these definitions, one may now focus upon establishing the scope within the context of modeling. Sections 1.2.2 and 1.2.3 establish this scope.

1.2.2 Modeling Ecosystems

To determine the environmental sustainability of an action, one must represent the action's impact on the environment, and to represent an action's impact, one must first possess a representation of the environment. This work uses ecosystem models to represent the environment. A lack of training and education in the fundamentals of biology and ecology prevents mechanical engineers from generating plausible ecosystem models. Therefore, this work depends upon ecosystem landscape models developed by systems ecologists from the Gund Institute of Ecological Economics at the University of Vermont (Costanza, et al. 1990;Costanza, et al. 2002). The selected models represent the culmination of nearly two decades of ecosystem modeling research. They capture hydrology, nutrient cycling, vegetation growth and decomposition, and they possess the ability to model ecosystems on multiple spatial and temporal scales (Costanza, et al. 2002;Voinov, et al. 1999a). Therefore, they form a strong foundation upon which to build a technical framework for estimating environmental impacts and assessing the sustainability of actions. But, representing the environment is only half the effort; one must also represent the economic actions that effect the environment.

1.2.3 Modeling Industry

Industrial and commercial goods contribute to the condition of being "well off," economic sustainability, stated in the working sustainability definition in Section 1.2.1. Creation of these goods directly affects the local and regional environment surrounding manufactories; so, this thesis limits consideration of economic sustainability to industrial sustainability within specified regions or locales. Within the context of the working definition, industrial sustainability is the ability of a facility or group of facilities to continue to or "preserve the capacity to" manufacture profitable products within a specified geographic area.

To explore the methods and consequences of continuing to manufacture profitable products, one must represent facilities. Representing facility behaviors requires the use of manufacturing models. These models capture key resource inputs and both intended and incidental (waste) outputs. Knowledge of these flows allows one to explore the consequences of different management decisions upon economic sustainability and environmental burdens.

1.2.4 Integrating Models

Based on the previous discussions about sustainability and modeling, one might begin to suspect that the task at hand is to redefine sustainability or create new and better models of ecosystems and factories. But, one must remember the goal statement forwarded at the beginning of Section 1.2. The objective is not to build new pieces. The objective is to assemble old pieces in a new way – to create a new technical framework by aggregation and integration of older models and frameworks.

In ecosystem modeling, human beings and their economic activities can be incidental. One can view human activity as a disturbance, albeit a recurring disturbance, of the non-sentient living system. An equivalent view holds for the industrial systems. Facility models with regulatory limits on emissions and resource consumption engender the view that the environment is a constraint, and occasional, successful violations of these constraints may convince the shortsighted that it is an artificial constraint. These technical perspectives sometimes lead to opposite, polarized views. Adopting the former, the most sustainable system is an uninhabited living system, and adopting the later, the most economical system is unregulated. Though both hold value, both are limiting. Creating new and better types of each may serve to further entrench the opposing camps.

Instead of fortifying one of the perspectives, this work focuses on the next logical step; this thesis focuses on linking the two types of models. Ecosystem and industrial models already exist; so, the work's contribution is combination. Creating, testing and evaluating the rudimentary elements of the interface between these model types are significant components of this work.

1.3 Questions for the Thesis

The previous sections witnessed the statement of an overarching motivation, the introduction of sustainability as a central theme and the narrowing of the scope of the thesis.

Section 1.1: Overarching Motivation
- Child's Question: 'How will one know when a locale or region attains a sustainable state?'

Section 1.2: Scope (*Introduction*)
- Statement of the thesis goal

Section 1.2.1: Sustainability Context and Relevance
- Defining Sustainability
- A Working Definition: Sustainability in the Context of this Thesis

Section 1.2.2: Modeling Ecosystems
- Value of ecosystem modeling with respect to the goal of the thesis

Section 1.2.3: Modeling Industry
- Value of industrial modeling with respect to the goal of the thesis

Section 1.2.4: Integrated Modeling
- Revealing integrated modeling as the means of achieving the goal of the thesis

Section 1.3: Questions for the Thesis
- Stating the questions that one must answer in order to successfully use integrated modeling to achieve the goal of the thesis

Figure 1-1: Diagrammatic View of the Development of the Motivation Underpinning the Thesis' Principal Questions

As shown in Figure 1-1, the previous sections progress from overarching motivations through a goal statement toward concrete objectives that support the goal of the thesis. Section 1.3 identifies and develops the research objectives implicit in Section 1.2.4. It focuses the work to a point by introducing the three principal questions addressed in the body of the thesis.

Integrating ecological and industrial models to determine environmental impact and assess the sustainability of an action or pattern of actions raises a host of questions. These questions fall into three categories: philosophical, technical and practical. The

philosophical questions deal with 'ought'; the technical questions deal with 'how.' The practical questions deal with results. As stated in the beginning of Section 1.2, part of the goal of this research is to 'specify…the fundamental building blocks…' for integrated 'industrial and ecological models.' So, the first question aims at stating the characteristics an eco-industrial model ought to possess. The second focuses on determining how to embody these characteristics because the goal statement calls for the unification of ecological and industrial models. The point of specifying and developing 'fundamental building blocks' is to establish a 'technical framework' capable of estimating environmental impacts. The third and final question prompts testing and evaluation to determine whether the embodied characteristics allow detection of ecosystem responses – environmental impacts.

Certainly, one document cannot contain the answer to the overarching motivational question forwarded in Section 1.1, but it can begin to investigate questions concerning the appropriate characteristics of linked models, technical means of integration and the resulting attention directing capabilities. These three topical areas yield the thesis' questions (See Table 1-1).

Table 1-1: Associating Primary Thesis Questions and Hypotheses with Chapters

Thesis Question	Hypotheses	Addressed In
1. What characteristics should linked industrial and ecosystem models possess?	1. An integrated model should include the dynamics, spatial pattern and local parameter variations of the surrounding ecosystem. It must include all significant mass and energy exchanges between the two systems.	• Chapter 2 – Literature Survey
2. How can one link ecological and industrial models?	2. Using STELLA and SME software, one can link the two types of models with mass exchanges and modifications to mechanisms and parameters.	• Chapter 3 – Forging Links
3. Can one currently detect the impact of industrial changes on the modeled ecosystems?	3. Yes, one can detect industrial effects as changes in landscape pattern and ecosystem function. Specifically, one can observe changes in nutrient loading and net primary production	• Chapter 4 – Testing and Evaluating Links

1.3.1 Thesis Question 1

One should determine the required characteristics of linked ecological and industrial models before endeavoring to resolve the associated technical problems. To predict environmental impacts and determine the sustainability of industrial actions, one must specify the characteristics of the technical framework which fulfills these needs. One way of beginning task clarification is to ask a series of related questions about the objectives behind different ways of integrating ecological models. The following inset contains one such set of questions – the thesis' first set of questions.

1. What characteristics should linked industrial and ecosystem models possess?

   a. What are the uses and resultant defining characteristics of current environmental and ecological models?

b. What are the uses and resultant defining characteristics of industrial

facility models?

c. What level of interaction do industrial facilities have with the

environment?

Each question in the first set aids in task clarification; answering each question helps identify the required characteristics of linked models. Researchers build models to understand phenomena and answer questions; so, the answer to Question 1a reveals the reasons that precipitated the creation of environmental and ecological models. One finds these reasons in Section 2.2. It also illuminates the important environmental model characteristics that one might wish to incorporate in an integrated model. The answer to Question 1b, found in Section 2.3, provides the same information for industrial models. Answering Question 1c identifies the critical relationships between industry and the environment. It serves as a filter for the characteristics identified by answering the first two sub-questions. The critical relationships which connect ecological and industrial systems are revealed in Sections 2.3.4 and 2.4. Taken together, these answers provide the characteristics from which one creates the specification for the desired framework.

1.3.2 Thesis Question 2

With a specification in hand, one proceeds to develop a technical framework that fulfills the clarified task. One builds the framework by linking industrial facility material / mass flow models with terrestrial ecosystem landscape models. Descriptions of these models appear in the second chapter. The thesis' second primary question and sub questions associated with linking these types of models follow.

2. How can one link ecological and industrial models?

    a. What inputs and outputs link the two types of models?

    b. How can one represent these links using available tools?

The answer to Question 2a is actually a formalization of part of the specification discussed in Section 1.3.1. Answering this question involves correlating system qualities with various system quantities. Question 2b further focuses the question by limiting the development of links to those capable of creation with available tools. The answer to the second sub-question is a draft of the technical framework. Besides serving as the first connection between the two model types, the draft serves as a demonstration of the malleability and limitations of existing model interface tools. During the course of answering these questions, one conceives and develops the essential elements of a technical framework for predicting environmental impacts and assessing the sustainability of actions.

1.3.3 Thesis Question 3

Once specified, designed and developed, one should test and evaluate the effectiveness of the framework. The third set of questions focuses on testing and evaluation; the third set focuses on results. The primary question and sub questions follow.

3. Can one currently detect the impact of industrial changes on the modeled ecosystems?

    a. Can one currently detect the impact of reasonable, industrial management decisions on the modeled ecosystem?

b. If so, what response patterns and trends appear, if any?

c. Do the predictions correlate with observed results or experience-based expectations?

d. Are model limitations encountered?

Changes in one facility or group of facilities may not induce noticeable responses in current ecosystem models. Since determining environmental impacts is foundational for this work, asking and answering question three are essential parts of the evaluation process. In fact, one may forgo, much to the detriment of the thesis, a great deal of evaluation, if changes in industrial systems are not found to impact the modeled ecosystems. To determine whether current ecosystem models can reveal the impact of industrial operations, hypothetical industrial disturbances are applied to an integrated model. Each specific disturbance is considered an experiment in which hypotheses concerning the response of the eco-industrial model are tested. Section 1.4 briefly discusses these experiments, and each experiment is discussed in detail in Chapter 4.

If changes to industrial systems actually influence current ecosystem models, one must explore the same question for more limited changes. For example, removing a facility or group of facilities from an ecosystem may not be an economically viable option. Question 3a aims at determining whether the framework can detect changes in ecosystems caused by smaller more controllable changes in industrial systems. Such smaller changes would include technological improvements or transitions and modifications in management practices. These changes would preserve the industrial system while potentially altering resource consumption and waste rejection.

If the ecosystem responds, spatial patterns and unexpected relationships among variables may manifest themselves. The purpose of Question 3b is to mandate searches for these data structures. One must observe and note these patterns for two reasons. First, the response of the highly nonlinear ecosystem model to various disturbances may reveal a general relationship between environmental impact and certain types of disturbances. Second, one can compare the simulated patterns and trends with those know to occur in real systems.

To accurately predict or direct attention to environmental impacts, one must confirm that the framework's results correspond to the behavior of actual ecosystems. Question 3c focuses on exploring the correspondence between real and modeled ecosystems. And, Question 3d, a related question, spurs investigation of discrepancies between simulated and real behavior. Taken together, questions 3 through 3d evaluate the ability of the design introduced in Section 1.3.2 to satisfy the specification mentioned in Section 1.3.1.

1.4 Experiments

Experiments provide a means of exploring the questions discussed in Section 1.3. Each experiment yields insight into one or more of the posed questions. Answering the second thesis question requires investigation of the topics listed in Table 1-2. Specification and embodiment of these links answers the second thesis question. Applying embodied links in experiments aids the reader's understanding of the answer. The experiments evaluate the functionality of the links; the results of the evaluations yield the answer to the third thesis question and its related sub-questions.

Table 1-2: Experiments and Rationale

#	General Experiment Topics	Rationale
1	Computational Links	Application and evaluation of computational controls
2	Inanimate Links	Application and evaluation of geo-physical connections
3	Animate Links	Application and evaluation of direct biosphere links

1.5 Organizing the Work

In the following four chapters, this document systematically addresses the themes and questions raised in the first chapter. The second chapter contains a literature survey the covering ecological modeling and industrial modeling. This effort serves to situate the thesis within the current body of work, and it contributes significantly to answering the first set of questions. Chapter Three develops the elements of the technical framework which accomplishes the goal of the thesis. Chapter Four contains a series of experiments that evaluate the technical framework elements. In these evaluations, one finds the answer to the third thesis question. The fifth and final chapter summarizes the answers to the thesis questions, reflects upon contributions and discusses future directions.

CHAPTER 2

Literature Survey – Context and Characteristics

Through the literature survey, the reader comes to understand the importance and requirements of eco-industrial modeling. Specifically, Chapter 2 exists to reinforce the motivation for this work and answer the first thesis question, 'what characteristics should linked industrial and ecosystem models possess?' An argument that demonstrates the relevance of the identified goal to the sustainability effort is formed in Section 2.1. Drawing from sustainability and modeling literature discussed in Sections 2.2 and 2.3, a list of fundamental requirements for eco-industrial modeling is created in Section 2.4. By establishing the requirements, one comes to understand the necessary and desirable characteristics of linked industrial and ecosystem models; one learns the answer to the first thesis question.

2.1 Sustainability and Eco-Industrial Modeling

The objective of Section 2.1 is to justify the importance of eco-industrial modeling to the sustainability effort using literature and thought examples. Section 2.1 exists to connect Sections 1.1's overarching motivation of predicting sustainable eco-economic states with Section 1.2's thesis goal of specifying and developing building blocks for eco-industrial models. Starting with Section 2.1.1, the connection is made by first casting industry's task of achieving environmental sustainability while preserving economic sustainability in terms of avoiding environmental constraints. In Section 2.1.1, one learns that the abstract concept of sustainability can be reduced to a set of constraints that one

can include in environmental and industrial models. Having defined the industrial sustainability problem in terms of avoiding constraints, Section 2.1.2 uses thought examples to detail two foundational limitations of current methods of addressing industry's problem. One learns that current methods lack the ability to guide mankind to a sustainable future. The section closes with a discussion of how eco-industrial modeling addresses the problem while overcoming the foundational limitations of current methods. While not contributing to the answer of the first thesis question, Section 2.1 provides a rationale for this work; it provides sound reasons why one should ask the thesis questions introduced in Section 1.3.

2.1.1 The Environment as a Constraint

Consulting literature that describes the requirements for a sustainable state is akin to reading the Ten Commandments found in the Judeo-Christian religious tradition. Sustainability guidelines and prohibitions tend to include some form of "thou shall" and "thou shall not" statements. This correspondence is not mere coincidence. Both sets of guidelines, on at least one level of abstraction, exist to aid in the self-governance of a system. In the former case, the system consists of a community of believers, and in the later case, the system consists of a community of socio-economic actors influencing ecosystem processes. Given the scope of this thesis, one can further narrow the community of socio-economic actors to a community of corporations with industrial facilities in a specific region or locale. The Ten Commandments limit or constrain some behaviors while setting minimum standards of achievement for others in a community of believers. Analogously, one may implement the various sustainability guidelines and prohibitions for a corporation or facility by viewing them as constraints, constraints that

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one may represent in a model. Norton emphasizes the need for determining the environmental constraints of larger systems in which smaller, managed systems are embedded (Norton and Hannon 1997). One may view a facility as constrained in the amount of a certain emission or as constrained to operate with a certain minimum efficiency, for example.

As mentioned, sustainability constraints often appear in the form of prohibitions, "thou shall not" statements, and required actions, "thou shall" statements. Speaking within the context of macroeconomics, Solow calls for society "to preserve the capacity to be well off" (Solow 1991). Hawken states that private enterprise must satisfy customers' needs and wants without degrading the environment's ability to satisfy future generations (Hawken 1993). The Brundtland sustainability definition stated in Section 1.2.1 makes similar demands. Moving beyond vague notions about capacities and inter-generational ethics, O'Riorden calls upon society to use renewable resources at replenishable rates, invest profits from non-renewable resources in renewable resource development, preserve life sustaining ecologies, "…redistribute essential liveability requirements…," ensure rights and monitor eco-socio-political change (O'Riordan 1996). To the growing list of sustainability imperatives, Wackernagel and Rees add the injunction not to allow pollution to exceed the sink capacity of natural systems (Wackernagel and Rees 1996). This short list reveals the manner in which industry receives guidance from sustainability researchers; it reveals that one can indeed express sustainability as a space bounded by constraints.

These pronouncements fall not upon deaf corporate ears. "…For a growing number of industries environmental issues are emerging with increasing frequency as strategic

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problems," and some global companies are incorporating environmental concerns into their strategic planning processes (Quazi 2001). Indeed, the World Business Council for Sustainable Development incorporates the sustainability concept into its mission statement ("About the WBCSD" 2003). Governmental regulators and concerned consumers pressure companies to meet environmental standards (Quazi 2001;Ramsey 2002). These actors give teeth to warnings about unsustainable actions. Incorporating eco-efficiency into strategic thinking allows firms to address environmental concerns, and for some, this action is partially taken to avoid the ire of regulatory and market actors (Michaelis 2003). So, whether from an appreciation of the future consequences of current environmentally unsustainable activities or from a fear of near-term consequences imposed by regulatory or market actors, companies tend to view sustainability guidelines and prohibitions as constraints.

Having fashioned sustainability guidelines into constraints, an important question arises. How can industry formalize these constraints? The preferred approach to formalization centers upon the identification of measures and creation of metrics that indicate the state of industry with respect to one of the constraints. Operating in accordance with the maxim, "What gets measured gets managed," some believe that knowledge of these metrics allows industries to manage themselves away from environmental constraints, given the necessary desire (Epstein and Wisner 2001;Schwarz, et al. 2002). However, knowledge of the eco-industrial state may not prove sufficient to steer a company clear of unsustainable activities in the long run. Using measures, metrics and indicators in this capacity is not without problems, as Section 2.1.2 reveals.

2.1.2 The Problems with Metrics Measures and Indicators

Two fundamental problems occur when one uses measures, metrics and indicators to guide a system toward a sustainable state. First and foremost, measures, metrics and indicators do not represent the underlying dynamics of a system. A simple numerical methods analogy illustrates this first problem. Secondly, measures, metrics and indicators restrict the vision of those involved in the decision process to the near term. An analogy to optimization reveals the potential folly of this short-sightedness.

To aid in understanding the first problem, take for a moment an omniscient perspective of the anthro-ecosystem that composes the living portion of planet Earth. From this vantage point, sustainability's meaning poses no intellectual difficulties. The imagined perspective reduces all uncertainties to probabilities, and the probability distributions are known. The reader is aware of every outcome in the past, present and future; rolls of the system's many "dice" bring no surprises. The appropriate characterization of the anthro-ecosystem's level of sustainability is known; moreover, the path of the system through time is also known. In fact, the omniscient observer may reduce the characterization of sustainability to a single variable function of time that one may easily graph (See Figure 2-1).
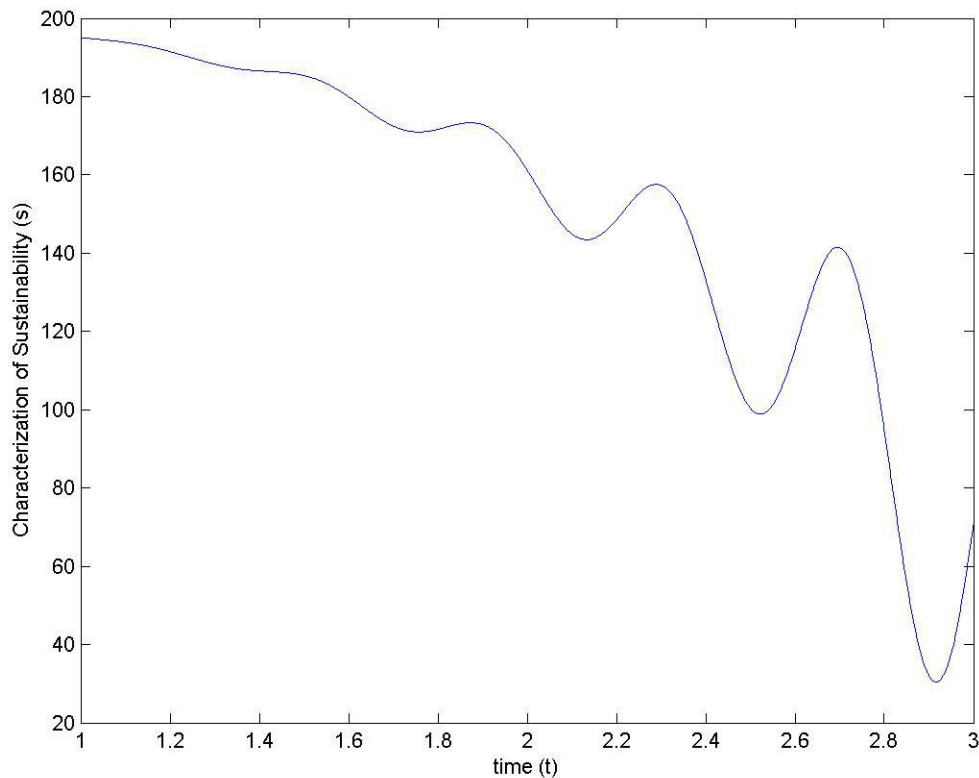
Figure 2-1: Sustainability vs. Time as Viewed from an Omniscient Perspective

Of course, mankind lacks the advantages of an omniscient perspective. To compensate, he attempts to represent or model the systems with which he interacts, and he uses these models to foresee the consequences of his actions. Enter measures, metrics and indicators. Frosch and coauthors consider environmental metrics at the "heart of how industry defines environmental performance" and estimates "progress" (Frosch, et al. 1999). Each measure, metric or combination of metrics and measures summarizes details about a system or component of a system. When they inform the viewer about the state of a system or component, they become indicators; they indicate the current or, more likely, past state of the system.

Even astoundingly accurate and precise summaries fail to predict future system behaviors, and they cannot directly reveal a system's underlying dynamics, unless the indicators are soundly founded upon these dynamics. Bereft of superior information, humanity often presses summaries into service as models representative of a system's governing dynamics. Figure 2-2 is a version of Figure 2-1 that compares hypothetical summary based "status quo" and recent "trend" estimates of system sustainability to true system sustainability. Summaries of the present become "status quo" predictions, and summaries from the recent past become predictions based upon "current trends." Unfortunately, the resulting representations are often lacking. This often leads to expectedly inaccurate predictions of future system states.
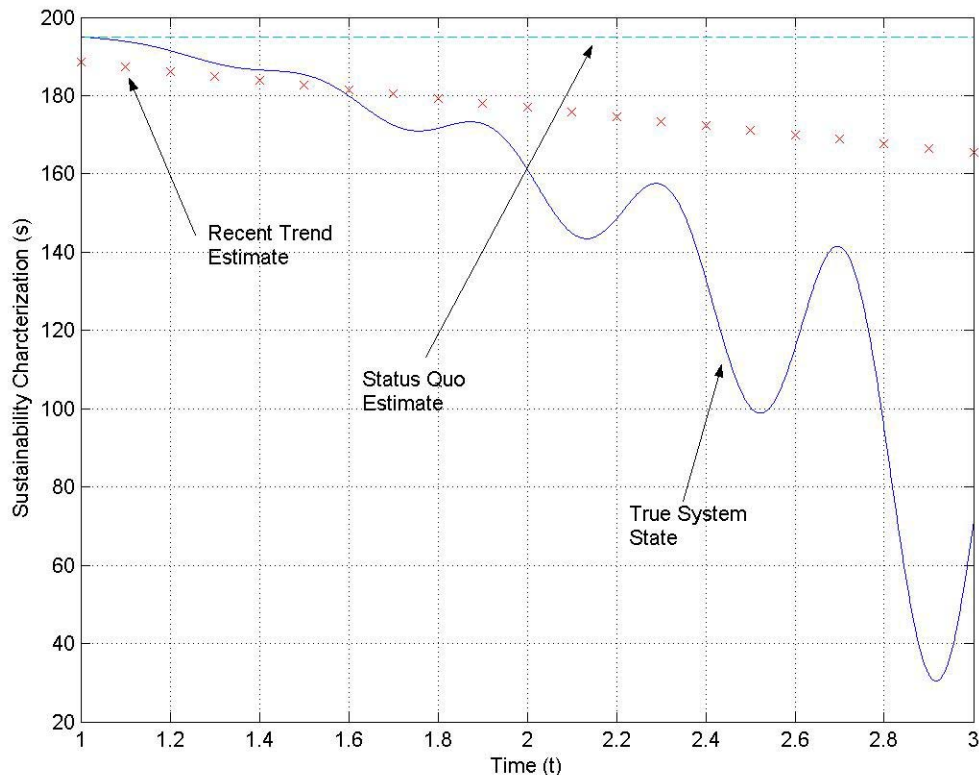
Figure 2-2: Estimating Sustainability Using Summary Indicators as Models

As Figure 2-2 shows, status quo and recent trend estimates both fail to predict the level of system sustainability as time progresses. The status quo estimate grows progressively worse with time, and the prediction based upon recent trends becomes increasingly inaccurate as previously minor dynamics manifest themselves to a greater degree. In short, summaries may represent, but they generally cannot predict.

To predict, one needs a model that captures or at least approximates the governing dynamics of the system. To know whether a decision or set of decisions drives a system toward or away from sustainability, one needs models that approximate a system's interrelationships, feedbacks and overall behaviors. The example from the omniscient perspective again illustrates the point (See Figure 2-3).
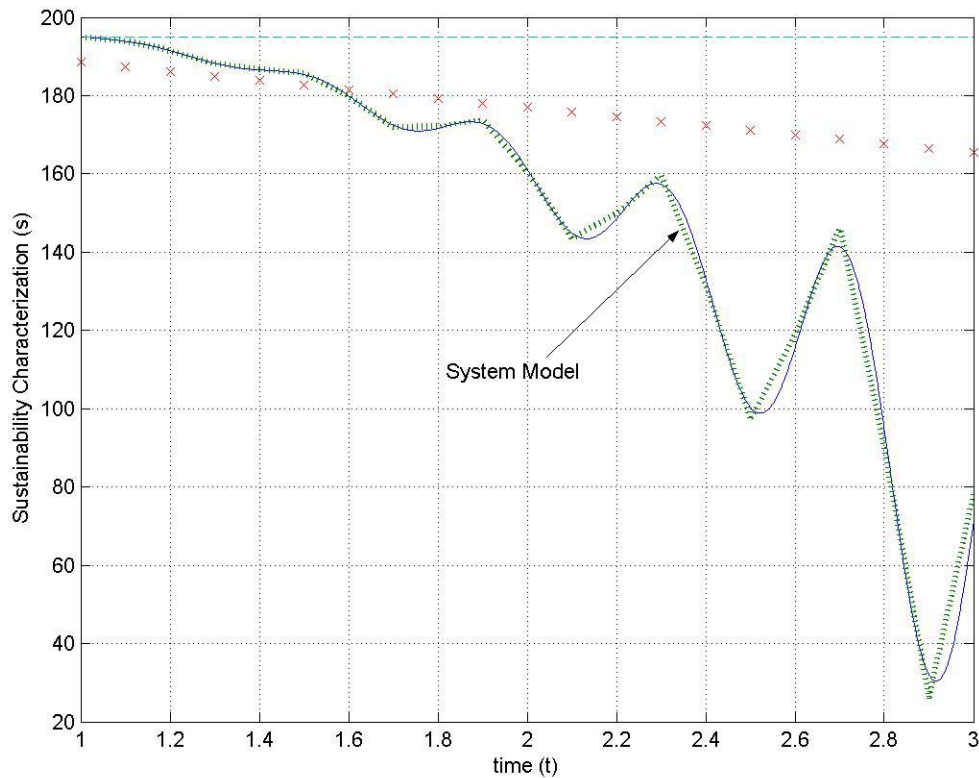
Figure 2-3: Estimating Sustainability Using an Anthro-Ecosystem Model

In Figure 2-3, a third order Taylor Series expansion called the "System Model" is used to approximate the fifth order polynomial with a sinusoid used to generate the hypothetical sustainability line. It successfully approximates the sustainability line because it includes information about the dynamics of the system. Specifically, it includes the first, second and third derivatives. The Taylor polynomial is analogous to a system model for industrial systems embedded in ecosystems.

One could glean measures and generate metrics from the mathematics underlying this simple example, and some of these measures and metrics might indicate something about the system. But, these potentially useful summaries are still simply summaries. They help turn data into information, and they assist in the organization of information. And now, one comes to the heart of the first fundamental problem with measures, metrics and indicators. Unless combined in a form equivalent to the Taylor Series expansion, they cannot predict the state of the system in the long term. Analogously, unless one combines industrial and ecological information in such a way as to represent eco-industrial system interrelationships, feedbacks and behaviors, one cannot predict the sustainability of the system.

Having identified the first fundamental problem with measures, metrics and indicators, one can focus on the identification of the second problem mentioned at the beginning of this section. The second problem results from the negative impact measures, metrics and indicators can have on the decision process. In a sense, the range of potential, yet unrealized, eco-industrial system states represents a design space. Continuing the analogy, a company's search for an economically and environmentally sustainable state

of operation represents the search for satisficing sets of operating parameters (Simon 2001). Management is the act of searching the space and researching the space as exogenous variables such as technology and average global temperature change. Consider the hypothetical environmental damage space presented in Figure 2-4. In the space, managers and designers control the two facility design variables, and they attempt to minimize the environmental impact of operations.
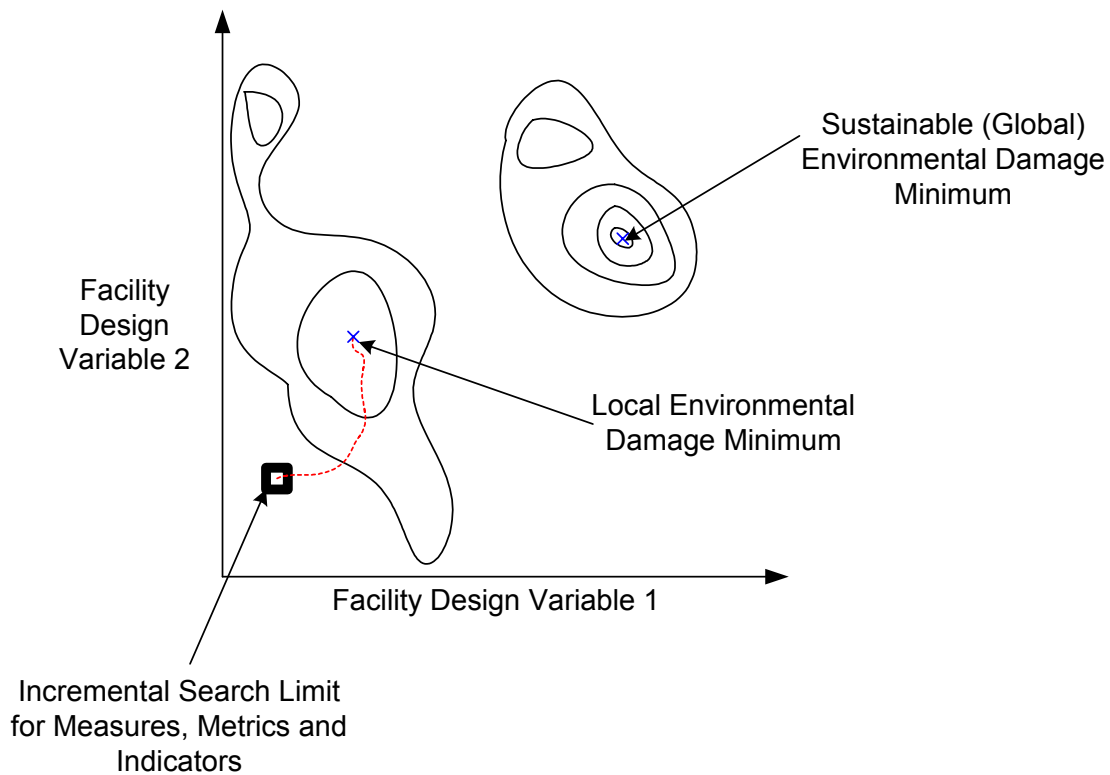
Figure 2-4: Two Dimensional Design Space with Environmental Damage Contours

However, the hypothetical managers are limited by the inability of measures, metrics and indicators to accurately represent the design space; the square with thick black lines in Figure 2-4 represents the limits of prediction for managers and designers using measures, metrics and indicators. The reader, benefiting from an omniscient perspective, can see the environmental damage contours, but the managers can only see what falls within the

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bounds of the square. Four environmental damage minimums are apparent, but only one of the minimums is global. If one assumes for the moment that one can achieve sustainable operations by changing the two design variables to the coordinates of the minimum, what is the likelihood of reaching the sustainable minimum through incremental improvement?

Given only accurate, current indicators or historically based trends in these indicators, decisions executed at comparatively small time steps to decrease the unsustainability of the system may lead to local eco-efficiency maximums or local environmental damage minimums which may fall short of sustainability, as the dotted line leading from the square to a local minimum in Figure 2-4 suggests. This careful incrementalism in the design process is the second fundamental problem with using only measures, metrics and indicators to guide design and development toward a sustainable outcome.

2.1.3 Goal: Testing Constraints Without Testing Constraints

For the human community to sustain itself, it must operate within the constraints imposed by nature. Violations, though "successful" in the near-term, inevitably lead to the degradation and collapse of ecosystems which provide complimentary natural services and capital. Preventing these dire consequences requires both will and understanding. Society must muster the will to work toward a sustainable state for the anthro-ecosystem, and scientists and technologists must provide the understanding of the system society wishes to sustain.

Knowledge of the impacts caused by industrial activities is part of the understanding requisite for sustainability under current global conditions. Those involved in various industrial decision processes need to know environmental constraints. They need to

approximate the sometimes unclear environmental results of their decisions before implementing them. Scientists and technologists need to provide a means of approximately predicting the behavior of eco-industrial systems. Indeed, the need for integrated modeling is already recognized by some within the context of natural resource management (Greiner 2004). With such approximations, responsible industrial parties could safely observe the results of their decisions within the context of a simulation. Here in lies the goal that this work advances. They could test the constraints imposed by the environmental component of the eco-industrial system without testing the constraints of the actual system.

2.2 Ecological and Environmental Modeling

Since eco-industrial modeling uses both environmental and industrial models, situating this work requires consideration of environmental and industrial modeling literature. Situation describes the uses and reveals the characteristics of current environmental models; situation answers thesis question 1a. The verb form of 'situate' means placement in a site or context, and this is exactly what Section 2.2 accomplishes. A two step process places the work within the *context* of the environmental modeling literature as illustrated by Figure 2-5.

Step 1: Providing Understanding

Step 2: Siting
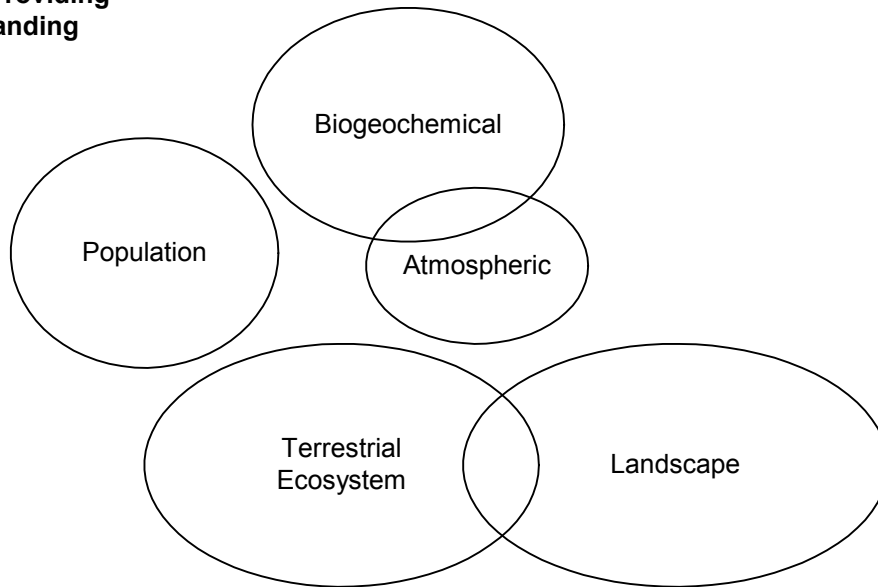
Ecological Modeling Foundation
for Eco-Industrial Modeling
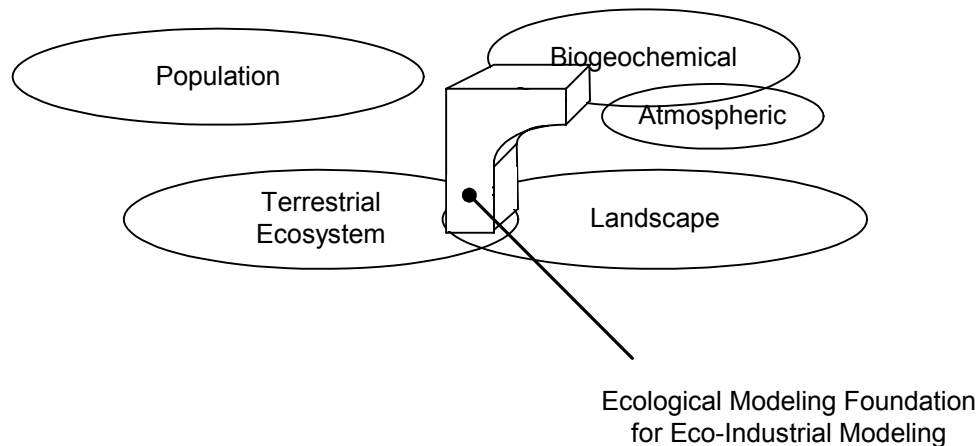
Figure 2-5: Diagraming the Primary Objectives for the Section

First, an overview of different types of environmental models is presented in order to provide the reader with a general understanding of environmental models and the reasons for creating them. During this overview, the state prediction and environmental impact estimation capacities of the models are given special emphasis. Then, ecosystem landscape models are selected as the *site* in the environmental modeling literature upon which the "eco" half of the eco-industrial modeling framework developed in this work.

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State and impact estimation capacities provide the core reasons for selecting ecosystem landscape models.

Jorgensen and coworkers provide an encompassing review of environmental and ecological models formulated prior to the mid-nineties (Jorgensen, et al. 1996). They organize the reviewed models by type and general purpose (See Table 2-1). Their reasonable classification scheme orders this discussion of ecosystem models.

Table 2-1: Environmental and Ecological Model Types and Purposes

#	Type	Purpose
1	Population	Animal population changes
2	Biogeochemical	Representation of aquatic ecosystem responses to flow and nutrient, chemical, heavy metal and / or radiological pollution
		Ecotoxicology
3	Atmospheric	Plume dispersion
		Air Pollution
		Acid rain
4	Terrestrial Ecosystem	Plant growth
5	Landscape Models	Analysis and prediction of changes in a region

2.2.1 Population Models

Population models are the oldest type of ecosystem models. In the mid-1920s, Lotka and Volterra developed models capable of representing animal population dynamics (Jorgensen, et al. 1996). Their analytical ordinary differential equation models qualitatively describe the population trajectories of single predator single prey systems (Boyce and DiPrima 1997). These models require inputs of initial population and predator-prey interaction parameters.

More sophisticated population models have since been formulated. For example, one model for smallmouth bass explicitly considers fish age, fish size, spatial location, prey availability, nesting sites and other variables when calculating population size

(DeAngelis, et al. 1991). One may simulate the impact of environmental burdens such as the introduction of toxins by modifying one or more of the considered mechanisms. The authors demonstrate this approach by changing the level of foraging activity and the growth mechanisms for smallmouth bass in response to the hypothetical introduction of a toxin (DeAngelis, et al. 1991). However, the model does not appear to contain a provision for modeling a toxin's means of acting upon these and other population governing mechanisms.

2.2.2 Biogeochemical Models

Biogeochemical models primarily exist to track the movement of nutrients and other materials within the hydrosphere and biosphere. They focus upon the "fate and transport" of these materials, and in some cases, they attempt to describe their impact on organisms. One example of a biogeochemical model focused upon representing aquatic ecosystem responses in the hydrosphere describes the "self-purification" of a biologically polluted river in France (Cazelles, et al. 1991). The model mathematically incorporates both the fluid mechanics and microbial action that determines the fate of dissolved organic carbon in a small river. One ecotoxicology model mathematically approximates the distribution of persistent organic chemicals in the atmosphere, hydrosphere, lithosphere and biosphere following release in southern Ontario (Patterson and Mackay 1989). The ultimate purpose of the model is to estimate the amount of organic chemicals in the human food chain and to thereby estimate the rate and sources of human absorption.

2.2.3 Atmospheric Models

Atmospheric models possess aims analogous to biogeochemical models, but they change media. Once again, the models focus upon the fate and transport of chemicals and nutrients; this fate and transport simply occurs in the atmosphere.

At the local level, this type of modeling centers upon plume dispersion. These models depend upon the mathematics of three dimensional Gaussian distributions or of heat transfer and fluid mechanics (Jorgensen, et al. 1996). Fisher and coauthors discuss the creation and evaluation of a plume dispersion model (Fisher, et al. 2001). This line of research seems to emphasize transport.

On a regional level, attention turns to what Jorgensen and coworkers describe as air pollution (Jorgensen, et al. 1996). Tropospheric ozone pollution is an example of regional air pollution. One representative article describes the structure of an ozone pollution model used to evaluate abatement strategies for the region surrounding Madrid, Spain (Palacios, et al. 2002). The model relates the release of nitrogen oxides and volatile organic compounds to the formation of ozone, and it predicts the ozone concentration in different parts of the region. As this example suggests, air pollution models balance consideration of transport and fate.

Atmospheric models also include the multi-regional scale phenomenon of acid rain. Butler and coauthors present a statistical acid rain model that correlates nitrogen oxide releases with nitrate precipitation (Butler, et al. 2003). As with air pollution models, the primary concern is to quantitatively link emissions with intermediate results. The impact upon living systems is not incorporated.

2.2.4 Terrestrial Ecosystem Models

Terrestrial ecosystem models include representations of agricultural and natural ecosystems. They specialize in estimating the response of these ecosystems or components of these ecosystems to specific types of changes. A model of olive tree growth in an orchard is an example of a basic agricultural terrestrial ecosystem model according to Jorgensen's classification (Abdel-Razik 1989;Jorgensen, et al. 1996). Though narrowly focused, the model relates olive tree function to changes in water and nutrient supply (Abdel-Razik 1989). Essentially, it quantifies the impact of a few environmental changes on olive orchards. Fitz and coauthors developed a more general model for natural terrestrial ecosystems which can also consider agricultural ecosystems (Fitz, et al. 1996). Their model includes nutrient cycles and ecological processes, and it simulates the response of plant communities to water, nutrients and other environmental inputs (Fitz, et al. 1996). In both presented cases, one should note that the impact upon plant growth and the responsible underlying processes are emphasized.

2.2.5 Landscape Models

Landscape models specialize in simulating changes in a region; spatial patterns and distributions are implicitly or explicitly included. For example, Malanson and coauthors simulate changes in vegetation for the Californian chaparral region as a result of changes in annual precipitation and mean temperature (Malanson, et al. 1992). The authors of this model implicitly model species distribution by considering it a function of precipitation and temperature (Malanson, et al. 1992). In this context, an explicit representation of distribution would include assignments of vegetation to a particular geographical location.

One is, however, not limited to models with ecological components. Jorgensen's broad definition for landscape models allows the inclusion of any of the previous types that contain a spatial dimension (Jorgensen, et al. 1996). One could conceivably label the previously mentioned Madrid ozone model a landscape model.

2.2.6 Ecosystem Landscape Models

Work published following Jorgensen's review contains a sixth model type – the ecosystem landscape model. In the structure prescribed by Table 2-1, these models represent a subclass of landscape models, but as a consequence of their importance to this work, they are considered separately. Ecosystem landscape models represent a fusion of terrestrial ecosystem models and landscape models. They derive their importance from the fact that they retain the properties of both. They describe small-scale ecosystem activities, and they simultaneously model larger scale spatial ecosystem patterns. This section reviews some important ecosystem landscape models. It also uses the literature to reinforce the importance of modeling both ecosystem processes and patterns.

Bossel and Krieger created a fine example of an ecosystem landscape model for tropical forests on the Malaysian Peninsula (Bossel and Krieger 1991). The duality of this type of modeling is present in their formulation and final model. The non-spatial, dynamic portion of their model centers upon the two related state variables of tree number and biomass (Bossel and Krieger 1991). These state variables depend directly and indirectly upon modeled ecosystem processes such as photosynthetic production, respiration, canopy transition, tree geometry, mortality and seed production (Bossel and Krieger 1991). However, the models lack hydrological and nutrient considerations. They create a spatial model by assembling their non-spatial, dynamic forest growth

models on a grid. They link their grid cells with probabilistically determined tree falls; "emergent" (large) trees in one cell may die and fall into an adjacent cell, thereby damaging and destroying parts of the adjacent canopy (Bossel and Krieger 1991). A biomass comparison for the non-spatial and spatially explicit forest models is of special interest. The authors observe a "pumping" of biomass levels in each tree growth stage for the non-spatial model, but for the spatial model, they observe an "approximate equilibrium" for biomass in the five modeled tree growth stages (Bossel and Krieger 1991). Spatial patterns have a significant impact upon ecosystem functions (Turner, et al. 2001). And, Bossel and Krieger's contrasting results highlight the importance of possessing tools capable of representing them.

Voinov and coauthors created the Patuxent Landscape Model (PLM) "…to simulate fundamental ecological processes on the watershed scale" (Voinov, et al. 1999a). To achieve a spatially explicit representation of an ecosystem, a modeled landscape "…is partitioned into a gird of square unit cells" (Voinov, et al. 1999a). A general ecosystem model (GEM) simulates the ecosystem dynamics within each cell (Fitz, et al. 1996). For the PLM, the cellular ecosystem models include a number of modules (See Table 2-2) (Voinov, et al. 1999a).

Table 2-2: Description of primary modules in the Patuxent Landscape Model (Voinov 1999)

Module	Description
Unit Cell Hydrology	Simulates the vertical flux of water within a unit cell
Nutrients	Simulates the cycling of nitrogen and phosphorus compounds within a unit cell
Macrophytes	Simulates the growth of plants within a unit cell
Dead Organic Decomposition	Simulates the decomposition of plant material within a unit cell
Spatial Surface Hydrology	Simulates the flow of surface water and nutrients (runoff, streams and rivers) among cells
Spatial Subsurface Hydrology	Simulates the flow of subsurface water and dissolved nutrients among cells

Software developed by Maxwell and Costanza link the modules in the GEM and the unit cells together (Maxwell and Costanza 1997).   One models different locations and ecosystems (i.e. forest, grassland, swamp, etc.) by changing parameters in the GEM and by inputting the appropriate data for the unit cell grid.   Figure 2-6 provides a highly abstract and schematic view of the described ecosystem modeling. It emphasizes the use of non-spatial ecosystem process models to capture the dynamics, and it illustrates the use of the unit cell grid in spatial modeling. Each tree represents a non-spatial ecosystem process model. Though the structure of models is the same in each grid square, the process models are parameterized for specific grid locations in the landscape.
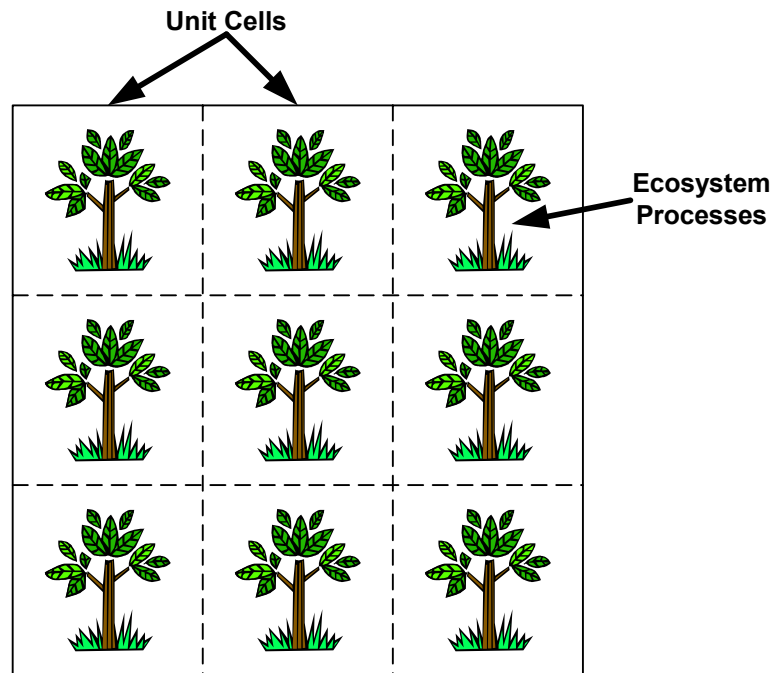
Figure 2-6: Abstract ecosystem landscape model

One constitutes a unit cell by combining an individual grid square with a parameterized process model. Figure 2-7 displays one of the stock and flow ecosystem process modules used in each unit cell. The module is implemented using STELLA modeling software. As one can see, the approach is analogous to a structural Finite Element Analysis where a structure is divided into (simplified) elements that can be analyzed and are connected using boundary conditions between the elements.
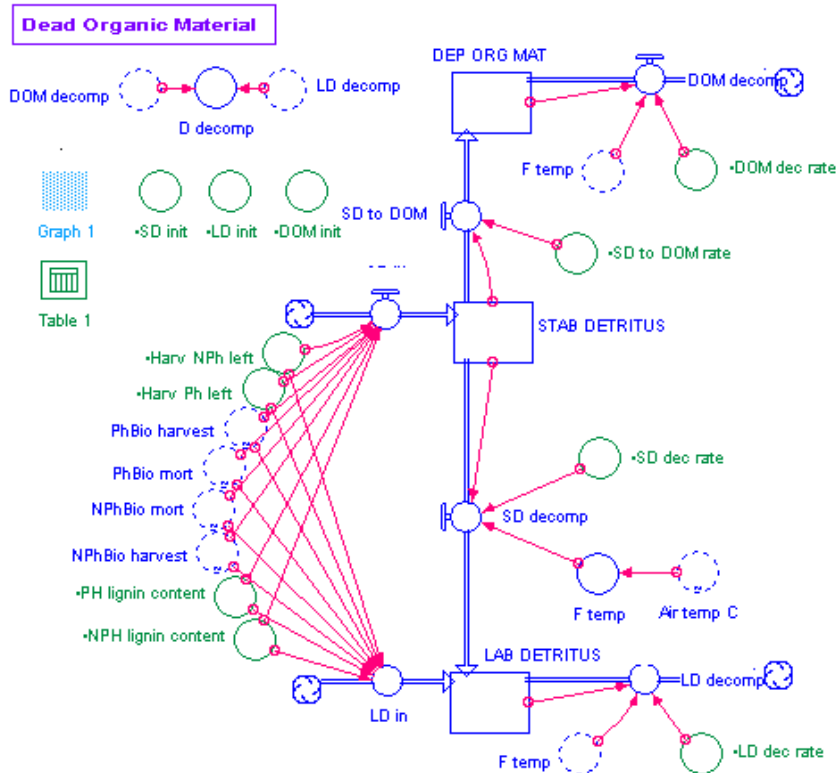
Figure 2-7: Dead Organic Material (DOM) ecosystem process model
(http://www.uvm.edu/giee/LHEM/)

The review highlights the power of ecosystem landscape models to represent both the dynamics and spatial patterns that govern ecosystem function. The discussed Malaysian Forest model revealed "pulsing" tree growth for a single square while manifesting an average equilibrium when multiple squares were linked into a spatially explicit model. PLM creation demonstrated the possibility of assembling multiple, non-spatial, dynamic unit models into a spatially explicit model capable of representing the hydrology, nutrient fluxes and biomass changes in local to small regional geographic areas. The review also serves to reveal the duality of structure common to this type of model. In the Malaysian Forest model, non-spatial dynamics are modeled using differential equations, and probabilistic tree fall events link the square regions represented by the non-spatially explicit differential equations. The PLM uses differential equation based unit models implemented in STELLA for non-spatial dynamics, and C++ user code links the unit

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models to form a spatially explicit ecosystem representation. In both cases, one sees the duality of the structure. Both the insight about dynamics and spatial patterns and the insight concering structure significantly influence the development of requirements for eco-industrial modeling discussed in Section 2.4.

2.3 Industrial Models

In a manner analogous to Section 2.2, this section situates this work within the context of the industrial modeling literature. Here, model types are classified, uses for the classified models are stated and model characteristics are revealed – answering thesis question 1b. Sections 2.3.1-2.3.4 use system type and model purpose to structure this survey of industrial models. As the sections progress, one comes to understand that not all industrial models are amenable to interaction with ecosystem models. Section 2.3.4 discusses models that hold the promise of being amenable. After viewing industrial models through the lens of system type and model purpose, one learns the reasons for building the industrial modeling foundation of eco-industrial modeling upon mass flow models.

Unfortunately, a survey of the literature failed to detect a sweeping industrial model survey analogous to the one used to structure the environmental and ecological model discussion in Section 2.2; so, a more fundamental though less specific discussion of modeling occurs in this section. Questions serve as the starting point for industrial modeling. The question of interest reveals the purpose and system of focus. Together, the purpose and focal system broadly define types of industrial models. When dealing with facilities that manufacture products, components and refined raw materials, these questions often revolve around material and / or energy flows. One models

manufacturing systems with the purpose of revealing opportunities (analysis) and creating situations (design) that increase system efficiency, minimize throughput times, decrease material and energy requirements, reduce waste, save money, comply with regulations and more. As one might imagine, different purposes lead to different models of the same system. However, the system also plays a part; different systems may require different sets of physical and mathematical principles. Different systems may require different models to achieve the same purpose.

2.3.1 Influence of the System

Physics and the continuity of product flow play an important role in industrial modeling. It is clear that different manufacturing processes require different models. The mathematical modeling of wire drawing is quite different than that for a petro-chemical distillation column for example. But, the continuity of product flow also plays a part. The particular manifestation of a manufacturing system depends upon production volume, product variety and product type (Askin and Standridge 1993;Hopp and Spearman 1996). Hopp and Spearman imply that different levels of volume and variety induce manufacturing facilities with different levels of product flow continuity (Hopp and Spearman 1996). For example, high variety, low volume production environments favor job shops while low variety, high volume environments favor well integrated assembly lines and continuous processing. These system contrasts lead to differences in model formulation because they require different physical principles and possess a different mathematical character. The principle of momentum conservation may be of little interest in a job shop, but it is important when considering fluid transport during continuous processing at oil refineries.

Some state that the mathematical characteristics of a model serve as a classification means (Hangos and Cameron 2001). The mathematics for modeling assembly lines and continuous processing differ in that assembly line modeling often mandates discrete considerations while continuous processing may require only continuous mathematics. One might reasonably represent material flows in continuous processing and on assembly lines as deterministic, but as a result of the variety in order type and timing, one would include stochastic elements in a job shop model.

Comparing job shops and assembly lines also highlights the manner in which distinct systems sometimes require distinct models to achieve the same purpose. In assembly line balancing, one of the objectives is to minimize idle time, and in job shop scheduling, one of the objectives is to minimize average completion time (Askin and Standridge 1993). One minimizes idle time subject to constraints by specifying the minimum number of required workstations, and one reduces average completion time by choosing the appropriate job start times on various machines (Askin and Standridge 1993). In both cases, the objective or purpose for constructing a model is to minimize wasted time in a material flow network, but as mention of the design variables reveals, the models are quite different.

2.3.2 Product Flow Network Models

Armed with an understanding of the influence of systems on models, one may proceed to consider the impact of intent. Systems engineering models often focus upon material, not necessarily mass, and accompanying information flows through networks. The nodes in the network often represent processes or waypoints in a manufacturing system. Commonly, the purpose of these models is to predict quantities such as

throughput, makespan, unit-time-in-system, work-in-process inventory, congestion, utilization, flexibility and quality (Askin and Standridge 1993). One uses this knowledge for tasks such as assembly line balancing, production scheduling, and general improvement or optimization of flow network efficiency and effectiveness (Askin and Standridge 1993).

These models focus primarily upon time and the movement of product. They apply within manufacturing system boundaries. Boundary crossing flows such as system wastes do not appear in the classical models, and even inputs appear to receive indirect treatment.

2.3.3 Manufacturing Process Models

Focusing on the individual nodes in a manufacturing material flow network, one enters the domain of engineering process models. The engineer models at this level to understand the physical transformation of inputs into outputs. What was simply an empirically determined time for the systems engineer expands into a microcosm for chemical and manufacturing engineers. When dealing with the manufacture of discrete parts and complete products, one encounters models for machining, welding, forging, rolling, forming, casting and more at the manufacturing process level (Kalpakjian 1997). These models depend upon fundamental principles such as Newtonian mechanics, material mechanics, mass conservation and the first law of thermodynamics. They also rely on empirical formulas such as Taylor's tool wear equation (Kalpakjian 1997). Continuous processing tends to fall into the domain of chemical engineering. Chemical process engineering models depend upon mass and energy conservation, reaction kinetics and fluid dynamics (Hangos and Cameron 2001). With their attention to first principles

and valid empirical relations, manufacturing process models can provide information about required inputs, desired outputs and the inevitable by-products. They can provide data about the mass, composition and energy content of these flows – data of interest when developing a physical interface with a system's surroundings. Unfortunately, the myopic attention to single processes poses a problem; the system level perspective is lost.

2.3.4 Mass and Energy Models

Manufacturing system level mass and energy flow models represent a compromise between the abstract product flow networks and narrow engineering process models discussed in Section 2.3.1. They are more concrete than product flow networks in the sense that they emphasize physical quantities. They are encompassing and more abstract than process models because they consider an entire system of processes at the expense of process detail. Eco-efficiency and environmental performance literature contains a significant body of work concerning this intermediate level of abstraction. Presence of this literature suggests the importance of manufacturing system level mass and energy flow models when considering industrial system interfaces with surroundings.

When considering the industry-environment interface from the industrial perspective, manufacturing system mass and energy flow model often appear. Allen and Shonnard describe methods for using "flowsheets," the authors' term for mass and energy flow models, to support pollution prevention and environmental performance assessment (Allen and Shonnard 2002). Bailey creates industrial mass flow models using input-output mathematics that one may apply on the national, multi-facility or single facility levels (Bailey, et al. 2001). The advantages of these steady-state models are that they allow the user to quantify various system mass flow efficiencies and they associate

system inputs and outputs on a per unit basis. Life cycle assessment guidelines call for the use of a mass and energy balance during the life cycle inventory phase of the assessment (Consoli, et al. 1993). And, Emblemsvag and Bras reengineered the activity based cost accounting framework to incorporate mass and energy flows (Emblemsvåg and Bras 2000). One significant advantage of this approach is that it traces mass and energy consumption to individual cost objects (often products) in the same way that standard activity based costing traces monetary costs; another advantage is that these models track waste mass flows (Emblemsvåg and Bras 2000). However, this type possesses the drawback that the relations between production and resource consumption are linear and empirical.

In Section 2.3.4, one sees the industrial half of the answer to thesis question 1c. One learns that mass and energy flows provide an important means through which industrial facilities interact with surrounding environments.

2.4 Extracting a Specification from the Literature

In this closing section of a chapter dominated by a survey of ecological and industrial modeling literature, knowledge gained during the review is used to answer the first thesis question. The essence of the models presented in Sections 2.2 and 2.3 is abstracted and used to formulate modeling requirements. Requirements for modeling ecosystem behavior mechanisms are forwarded; then, requirements for industrial models capable of interfacing with the natural environment are advanced. Design literature provides guidelines for design specification creation (Pahl and Beitz 1999). These guidelines structure the formulation of the mentioned modeling requirements. Finally, the two

resulting requirements lists are combined to form a list containing the characteristics for eco-industrial models – the answer to the first research question.

2.4.1 Specifications for Modeling Ecologies

Informed by the review in Section 2.2, one may create a general list of requirements for ecological modeling. Since this list precedes the creation of a technical framework for eco-industrial modeling, a design perspective is appropriate. Pahl and Beitz provide guidelines for specification generation in mechanical engineering design (Pahl and Beitz 1999). One may modify these guidelines to create a requirements list structure for ecological modeling. In this section, a modified design specification structure and ecological modeling knowledge unite to form an ecological modeling list of requirements.

Mechanical engineering design guidelines contain a list of seventeen general headings for requirements lists (Pahl and Beitz 1999). However, not all of these apply to ecological modeling. Table 2-3 contains the original set and a vetted set for ecological modeling.

Table 2-3: Requirements List Heading for Ecological Models

Requirements List Headings	Mechanical Design	Ecological Modeling	Meaning in Context of Ecological Modeling
Geometry	Yes	Yes	Spatial dimensions of a landscape (area covered, canopy height, etc.)
Kinematics	Yes	Yes	Rate and change in rate of material transfers in biogeochemical cycles and components of these cycles
Forces	Yes	Yes	Same as engineering
Energy	Yes	Yes	Representation of the influence of sunlight (temperature, photosynthesis, etc.)
Material	Yes	Yes	The building blocks of ecosystems and materials introduced by mankind (Biomass, nutrients, toxins, etc.)
Signals	Yes	*No*	*Data passed between organisms (chirp of bird, insect pheromones etc.)*
Safety	Yes	*No*	*Ecosystems do not develop with the safety of humans in mind*
Ergonomics	Yes	Yes	Intuitiveness of interface with the model
Production	Yes	*No*	*Creation of biomass; better represented under other headings*
Quality Control	Yes	Yes	Verification and validity of the components of a model
Assembly	Yes	Yes	The ability to add and subtract model functions
Transport	Yes	Yes	Implementation of the model on multiple computer platforms
Operation	Yes	*No*	Ability to control and manipulate the model; better covered by other headings
Maintenance	Yes	Yes	Updating software and modules
Recycling	Yes	*No*	*Cycling of materials in the ecosystem; better represented under other headings*
Costs	Yes	*No*	*Quantified anthropogenic value does not influence ecosystems*
Schedules	Yes	*No*	*Ecosystems do not operate on anthropogenic time tables*

The headings for signals, safety, production, operation, recycling and costs are not needed on an ecological modeling requirements list. Natural systems include a multitude of signals from the chirp of a bird to insect pheromones, but the level of aggregation in the surveyed ecosystem models is such that they account for these signals using ecological processes. For example, predator-prey models include a mortality rate for the prey. The ability of the predator to see, hear, smell and feel its prey must influence this mortality. An able-bodied rabbit would be reasonably safe from a blind and deaf fox after all. One could stretch the definition of production to apply to the surveyed models; one could discuss the production of biomass in a terrestrial ecosystem model for example. However, such quantities are better described as rates of material flows under other headings. Nature did not evolve with safety in mind, and operations and costs are also inherently anthropogenic concerns that do not influence ecosystems. Finally, the recycling heading is redundant in that tracing rates and materials reveals the cycling and loss of materials in an ecosystem.

Remaining headings possess useful interpretations for the design of ecosystem models; such headings reveal the environmental half of the answer to thesis question 1c. Geometry requirements in ecosystem models are analogous to requirements to represent spatial dimensions. The existence of the landscape and ecosystem landscape models discussed in Sections 2.2.5 and 2.2.6 reveals the importance of geometric requirements. The discussions in these sections reveal that including spatial considerations changes model output. For example, the inclusion of spatial considerations in the Malaysian Forest model results in a change in predicted tree growth behavior from "pulsing" to equilibrium (Bossel and Krieger 1991). Kinematics deals with velocities and

accelerations. These considerations are of value when dealing with the influence of transport phenomenon and other fluid mechanics phenomenon on water quality as mentioned in Section 2.2.2. The rate of material transfers is also important for the terrestrial ecosystem, biogeochemical and toxicology models reviewed in Sections 2.2.2, 2.2.3 and 2.2.4. Since these types of models include material transfer rates, one must include them in any general list of requirements for ecosystem models. The transfers may occur between the modeled system and the system's environment as illustrated by water transfers in Abel-Razik's olive orchard model (Abdel-Razik 1989), or the transfers could occur between different "compartments" in the same model, as illustrated by the movement of toxins in Patterson and Mackay's ecotoxicology model (Patterson and Mackay 1989). A general model must allow both types of transfers. Forces directly and indirectly influence ecosystem models. Water quality models that include fluid mechanics, such as the one developed by Cazelles and coauthors (Cazelles, et al. 1991), require the direct modeling of forces while some models incorporate the influence of forces in ecosystem processes. Energy drives both artificial and natural systems. The terrestrial ecosystem models presented in Section 2.2.4, landscape models in Section 2.2.5 and ecosystem landscape models in Section 2.2.6 possess a means of representing the transformation of radiant inputs into chemical energy and eventually biomass by photosynthesis. So, one must add the requirement to account for radiant inputs to those summarized in Table 2-4. The reviews of biogeochemical, toxicology and terrestrial ecosystem models in Sections 2.2.2, 2.2.3 and 2.2.4 revealed the need to account for materials in the form of nutrients and / or toxins in environmental models, adding two more requirements to the growing list. Materials such as nutrients and toxins require a

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carrier material that one must also take into account. The plume dispersion models mentioned in Section 2.2.3 highlight the importance of accounting for carrier materials.

Headings such as ergonomics, maintenance, assembly, transport and quality control deal with the use and support of the model. Requirements associated with these headings come from experience working with a component of the PLM discussed in Chapter 3. Ideally, the model would be ergonomic and readily maintainable; using it would be intuitive. One would also want to build only as much complexity as necessary into a particular ecosystem model; so, an ecosystem modeling structure designed to allow the addition and subtraction of functionality is desired. Transport refers to the ability to implement the model on multiple platforms. Since transferring ecosystem landscape models between platforms has proved a painstaking and time-consuming task, platform independence is desirable, and support on common computer platforms is required. Quality control in modeling refers to the verification and validity of a model's components. Before using models to support decision processes, one must, to the extent possible, establish model validity and appropriateness. Table 2-4 summarizes the headings and associated requirements.

Headings	*D*emand / *W*ish	Requirements
Geometry	D	Variation in three spatial dimensions must be considered
Kinematics	D	Rate of material input and output must be considered
	D	Rate of material transfer between components of the model must be included
Forces	W	Important for model components dependent upon a first principles analysis of fluid flow
Energy	D	Radiant inputs required for photosynthesis
	D	Other thermal inputs required to determine ecosystem health
Materials	D	Nutrients must be included
	D	Toxins must be included
	D	Carrier materials (water, air) must be modeled
Ergonomics	W	Intuitive interface, easy to use
Quality	W	Assumptions clearly documented
Control	D	Valid for intended purpose
Assembly	D	Must be capable of adding and subtracting functionality at will
Transport	W	Implementation should be computer platform independent
	D	Implementation must be compatible with common computer platforms
Maintenance	D	Data structures must be easily accessed, edited and augmented

2.4.2 Specifications for Modeling Industrial Facilities

In a manner similar to the previous section, one can draw upon the review in Section 2.3 to build a list of requirements for industrial modeling. First, the Pahl and Beitz list is modified with an eye to the goal of interfacing industrial models with ecosystem and environmental models. Then, the modified list joins with insights gleaned from the literature to form a list of requirements.

Headings for signals, safety, operations, recycling costs and scheduling are not needed in lists of requirements for industrial models meant to interface with ecosystem models. Table 2-5 indicates the headings of use in industrial modeling.

Table 2-5: Requirements List Headings for Industrial Modeling

Requirements List Headings	Mechanical Design	Industrial Modeling
Geometry	Yes	Yes
Kinematics	Yes	Yes
Forces	Yes	Yes
Energy	Yes	Yes
Material	Yes	Yes
Signals	Yes	*No*
Safety	Yes	*No*
Ergonomics	Yes	Yes
Production	Yes	Yes
Quality Control	Yes	Yes
Assembly	Yes	Yes
Transport	Yes	Yes
Operation	Yes	*No*
Maintenance	Yes	Yes
Recycling	Yes	*No*
Costs	Yes	*No*
Schedules	Yes	*No*

Signals and schedules are important for the product flow network models discussed in Section 2.3.2, but as discussed, these models lack a physical link to their surroundings. Therefore, these headings are not important for industrial models that must interface with the environment. A mathematical or simulation model is not a product capable of harming someone in and of itself; so, a safety heading is not needed. The operation heading typically includes requirements about the environment in which one expects a product to operate (Pahl and Beitz 1999). Given the required level of detail and the fact that the industrial model is destined to interface with a model of its environment, the operation heading is unnecessary and redundant. As made evident in Section 2.3.4, materials and flow rates are an important component of models amenable to interfacing with ecosystem models, but the recycling heading is redundant because other headings provide for similar material and flow requirements. Finally, the interface between two

physical systems does not change if one or more components of either system changes in dollar value. The fiction of dollar value is at best a dependent variable, and as a result, consideration of costs is unnecessary.

The remaining headings hold value for industrial model specification creation. Terrestrial ecosystem landscape models such as the PLM discussed in Section 2.2.6 assign ecosystem types to square areas on a grid of the modeled landscape (Costanza, et al. 2002). These grid areas have specified sizes. When the scale of the modeled industrial facility approaches the ecosystem model's spatial resolution threshold, the geometry (i.e. footprint) becomes important. One must consider the creation of a "built" or "industrialized" ecosystem type in such a case. Geometry is also important if one models multiple facilities. The importance of the mass flow models reviewed in Section 2.3.4 underscores the importance of knowing flow rates – a kinematics based requirement. In fact, Bailey's industrial input / output modeling method is based solely upon understanding rates (Bailey, et al. 2001). The inclusion of force depends upon the detail demanded by the industrial modeling activity. Detailed models meant for process redesign, such as those in Section 2.3.3, may need to consider forces, but models focusing on mass and energy flows between activities would not. Accounting for energy flows is a useful activity in and of itself, and thermal pollution secures its place as part of an industrial model meant to interface with the environment. The materials heading contributes multiple requirements to industrial model specifications. One must know the main types of materials exchanged between the processes and between the system and its environment. One must also quantify the amounts. These requirements come from the use of mass and energy flow models such as Allen and Shonnard's "flowsheets" in

pollution prevention and environmental assessment activities (Allen and Shonnard 2002). Identification of input and output material types and quantification of amounts are also key components of life cycle assessment (LCA). Production drives the mass and energy flows in a facility; so, an industrial model must possess the capability to vary production levels.

Table 2-6: Requirements List for Industrial Modeling

Headings	*D*emand / *W*ish	Requirements
Geometry	D	Must include footprint when near spatial scale of the ecosystem model's minimum resolution
	D	Must include locations when modeling multiple facilities
Kinematics	D	Rate of material input and output must be considered
	D	Rate of material transfer between components of the model must be included
Forces	W	Needed only detailed manufacturing process descriptions
Energy	D	Must account for heat outputs to the environment
	W	Should account for energy consumption in activities
Materials	D	Must include input types
	D	Must include output types
	D	Must include flows between manufacturing processes
Ergonomics	W	Intuitive interface, easy to use
Quality Control	W	Assumptions clearly documented
	D	Valid for intended purpose
Assembly	D	Must be capable of adding and subtracting functionality at will
Transport	W	Implementation should be computer platform independent
	D	Implementation must be compatible with common computer platforms
Maintenance	D	Data structures must be easily accessed, edited and augmented

Finally, the remaining headings of ergonomics, quality control, assembly, transport and maintenance hold the same meanings for industrial models as for ecological models. Their associated requirements apply to both types of models. The industrial modeling requirements are summarized in Table 2-6.

2.4.3 Requirements List for Eco-Industrial Modeling

Having completed ecological and industrial modeling literature reviews and having assembled requirements lists for each, one holds the essence of the answer to the first thesis question. The requirements for each type of modeling are synonymous with the desired characteristics for each type. Combining these lists creates an eco-industrial modeling requirements list (See Table 2-7). This list contains the necessary and desirable characteristics of eco-industrial models; this list is the answer to the first thesis question.

Table 2-7: Eco-Industrial Modeling Requirements List

Headings	*Demand* / *W*ish	Requirements
Geometry	D	Variation in the three spatial dimensions must be considered
	D	Must include facility footprint when near spatial scale of the ecosystem model's minimum resolution
	D	Must include locations when modeling multiple facilities
Kinematics	D	Rates for material inputs and outputs crossing the ecosystem model's boundaries must be considered
	D	Rate of material transfer between ecosystem stocks must be included
	D	Rate of material input to and output from the facility model must be considered
	D	Rate of material transfer between processes in the facility model must be included
Forces	W	Important for model components dependent upon a first principles analysis of fluid flow
	W	Needed only for detailed manufacturing process descriptions
Energy	D	Radiant inputs required for photosynthesis
	D	Must account for heat outputs to the environment
	W	Should account for energy consumption in activities
Materials	D	Nutrients must be included
	D	Toxin must be included
	D	Carrier materials (air, water) must be included.
	D	Must include facility input and output types
Ergonomics	W	Intuitive interface, easy to use
Quality Control	W	Assumptions clearly documented
	D	Valid for intended purpose
Assembly	D	Must be capable of adding and subtracting functionality at will
Transport	W	Implementation should be computer platform independent
	D	Implementation must be compatible with common computer platforms
Maintenance	D	Data structures must be easily accessed, edited and augmented

The requirements list presented in Table 2-7 contains the necessary and desirable characteristics of eco-industrial models. One can use the list to support the hypothesized answer to the first thesis question. One can also select the ecosystem and industrial

models to link to form an eco-industrial model by comparing characteristics of different environmental and industrial models with the listed requirements. In what follows, the hypothesized answer to the first thesis question is supported using the information in Table 2-7. Selection of the component models for an eco-industrial model is deferred until Chapter 3.

In Chapter 1, it was hypothesized that 'a linked model should include the dynamics, spatial pattern, and local parameter variations of the surrounding ecosystem,' as well as 'all significant mass and energy exchanges between the two systems.' One extracts four focal themes from this hypothesis: system dynamics, spatial patterns, local parameters and mass and energy exchanges.

Dynamics	Spatial Patterns	Local Parameters	Mass and Energy Exchanges
- *Kinematics* (both industrial and ecosystem) - *Forces*	- *Geometry* (3-D variations)	- *Geometry* (3-D variations, facility footprint, facility location)	- *Kinematics* (both industrial and ecosystem) - *Energy* (radiant inputs as well as consumption and thermal pollution) - *Material* (nutrients, toxins, carriers and raw materials)

Figure 2-8: Affinity Diagram Associating Requirements List Headings with Focal Themes

As shown in Figure 2-8, the seven requirements list headings related to the representation of the physical system can be grouped beneath the four themes found in the hypothesized answer to the first thesis question. This fact supports the hypothesized answer to the first thesis question.

With the first thesis question answered and the first hypothesis supported, the way is clear to select and link ecosystem and industrial models. In the third chapter, these two

activities occur. Characteristics from the eco-industrial modeling requirements list are used to select the appropriate models to link, and the mechanics of linking the models are outlined.

CHAPTER 3

Connecting Ecosystem Landscape and Industrial Mass Flow Models

The primary objective in Chapter 3 is to answer the second thesis question, 'How can one link ecological and industrial models?' Before creating links, one must identify the ecosystem and industrial models that one wishes to link. So, the chapter begins with the identification of industrial mass flow models and ecosystem landscape models as the two types of models most capable of satisfying the eco-industrial modeling requirements listed at the end of Chapter 2. Having identified the appropriate models, the chapter proceeds to conceptualize the linkages between ecosystem and industrial models. These links and the process of creating them serve as the answer to the second thesis question.

3.1 Identifying Components for Eco-Industrial Models

In Section 3.1, ecosystem landscape and industrial mass flow models are identified as the appropriate component models for eco-industrial models. The selection is based on a mapping of the requirements stated in Section 2.4.3 to the functions offered by models and model types reviewed in Sections 2.2 and 2.3. After mapping requirements to available functions, the computational infrastructure supporting the models used in this work is described in Sections 3.1.2 and 3.1.3. Section 3.1 partially answers question 2a by identifying the ecological and industrial models one should link to form an eco-industrial model. One finds the remainder of the answer to 2a in Section 3.2.

3.1.1 Mapping Requirements to Models

Of existing environmental and industrial models, ecosystem landscape and industrial mass flow models fulfill the most requirements on the list in Section 2.4.3. Figure 3-1 connects physical requirements with the model types and components that fulfill them.

Requirements | **Embodiments**

Rate of material transfer between ecosystem stocks must be included

Nutrients must be included

Radiant inputs required for photosynthesis

Toxins must be included

STELLA modules representing ecosystem dynamics (plant growth, nutrient cycling, etc.)

Carrier materials (air, water) must be included.

Rates for material inputs and outputs crossing the ecosystem model's boundaries must be considered

Ecosystem Unit Model composed of multiple STELLA modules converted to C++ code and joined by the SME

Must include facility footprint when near spatial scale of the ecosystem model's minimum resolution

Variation in the three spatial dimensions must be considered

Discretized local landscape composed of unit models connected by surface and subsurface hydrology algorithms

Must include locations when modeling multiple facilities

Rate of material input to and output from the facility model must be considered

Mass / material flow models for facilities and systems in facilities

Rate of material transfer between processes in the facility model must be included

Must include facility input and output types

Figure 3-1: Mapping of Requirements to Model Embodiments

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The first three labeled embodiments in Figure 3-1 are components of a particular ecosystem landscape model; specifically, the components are parts of the ecosystem landscape modeling framework devised by Costanza and coworkers(Costanza, et al. 2002). The fourth labeled embodiment is a generic representation of a mass flow model for an industrial facility that accounts for facility inputs and outputs as well as inter-process flows.

Consider the first three components in Figure 3-1 and the associated requirements. STELLA modules fulfill requirements to account for nutrients, toxins and carrier materials. These modules also account for ecosystem processes such as material cycling within a unit cell and plant growth. The modules combine to form a complete representation of the ecosystem in a specified unit area. Combination connects carrier materials such as water with carried materials such as nutrients. The definition of a unit cell establishes a boundary across which input and output materials flow – fulfilling the second requirement opposite the unit model. By changing modules and parameters, one creates different habitats; the ability to create different habitats through combination and parameterization allows representation of industrialized "habitats." Requirements to represent variations in habitat patterns as well as the locations of industrial facilities are fulfilled using a discretized landscape composed of unit models. The discretized landscape allows different ecosystems (unit models) in each grid square. By assembling different unit models, one approximates the spatial ecosystem patterns observed in a landscape. Each grid square can also serve as the location for a factory.

The fourth embodiment symbol in Figure 3-1 represents a class of models that have the representation of mass flows in common. Models of this type were discussed in

Section 2.3.4. These models typically account for one or all of the significant material flows into and out of a manufacturing facility. Some account for flows within the facility. Therefore, they can fulfill requirements related to identifying and quantifying material flow rates on the facility and process levels.

Two sets of requirements do not appear in Figure 3-1: unfulfilled physical requirements and computational infrastructure requirements. Of the unfulfilled physical requirements, three are wishes. The unfulfilled demand pertains to the estimation of environmental impacts resulting from thermal pollution. Consequently, an eco-industrial model based upon Costanza and company's ecosystem landscape model framework and mass flow models would be a less than ideal choice for modeling facilities with large thermal outputs. Table 3-1 contains comments on the status of the selected models with regard to the computational infrastructure requirements.

Table 3-1: Assessing Fulfillment of Computational Requirements for Eco-Industrial Modeling

Computational Requirement	Yes / No	Comment
Intuitive interface, easy to use (W)	No	-
Assumptions clearly documented (W)	Yes	The physical assumptions are clearly documented though somewhat scattered.
Valid for intended purpose (D)	Yes	Ecosystem and mass flow models have been validated.
Must be capable of adding and subtracting functionality at will (D)	Yes	Ecosystem unit model assembled from STELLA modules
Implementation should be computer platform independent (W)	No	-
Implementation must be compatible with common computer platforms (D)	Yes	Compatible with Unix / Linux; NOT compatible with MS Windows standard
Data structures must be easily accessed, edited and augmented (D)	Yes	Provided that all necessary software is available, data structures can be accessed, edited and augmented.

As one can see, the computational necessities of eco-industrial modeling are fulfilled by the discussed model combination. Coupling these types of models would, therefore, create a linked model with a majority of the characteristics of an ideal eco-industrial model.

3.1.2 Describing STELLA

In this section, the structure of the STELLA software and its use in ecosystem landscape modeling are discussed. STELLA is an iconographic differential equation system creation and solution tool developed by isee Systems™ (formerly High Performance Systems) to facilitate simulation and modeling in education, business, government and research. Costanza and company use STELLA to create representations of ecosystem dynamics in unit cells (Costanza, et al. 2002).

The STELLA software has two functions. First, it supports differential equation based model creation, and second, it solves the created system of differential equations numerically. The software most successfully embodies the first function. Differential equation based model creation is supported using a graphical user interface that presents states, rates and parameters using three basic icons: "stocks," "flows" and "converters" (See Figure 3-2).

Stock - an accumulation

Flow - change in an accumulation per unit time

Converter - term modifying a stock, flow and / or other parameter
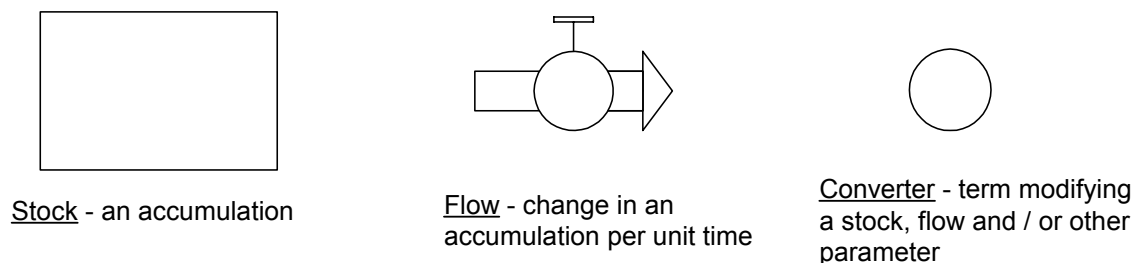
Figure 3-2: Basic STELLA Icons

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The software also accommodates data inputs and discrete events, though additional icons are used in the later case. One links groups of icons to form differential equations and systems of differential equations. For example, one could use STELLA to determine the mass at any given point in time in a system governed by the equation $\frac{dm_{sys}}{dt} = m_{in} - m_{out}$. One represents the familiar conservation of mass equation in STELLA by adding two "flows" to a "stock" (See Figure 3-3).
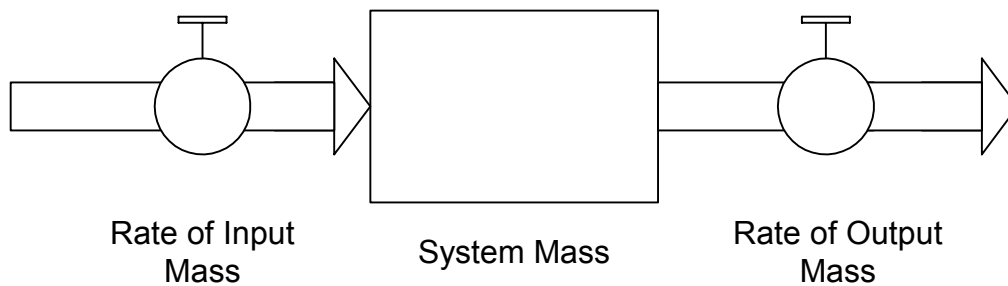
Figure 3-3: Conservation of Mass Equation Written Using STELLA Icons

As mentioned, the flows could be constants, equations based on stocks, flows and parameters or even empirical data contained in tables. Once a system is encoded using STELLA icons, one utilizes numerical methods integrated into the STELLA software to solve the differential equations. The software uses versions of Euler's Method and Runge-Kutta to solve the systems of differential equations.

In this work, STELLA is used in two ways. It is the environment in which Costanza and coworkers programmed the dynamics for the individual grid squares in their ecosystem landscape models as noted in Section 2.2.6 (Costanza, et al. 2002). So, it is used to represent ecosystem processes on 200 m^2 to 1 km^2 scales. Table 3-2 contains a list of major ecosystem processes represented by STELLA modules. Inputs to these

models include initial values, ecosystem process parameters and arrays of ecosystem, climate and geography data.

Table 3-2: Ecosystem Process Represented by STELLA Modules

Module	Description
Unit Cell Hydrology	Simulates the vertical flux of water within a unit cell
Nutrients	Simulates the cycling of nitrogen and phosphorus compounds within a unit cell
Macrophytes	Simulates the growth of plants within a unit cell
Dead Organic Decomposition	Simulates the decomposition of plant material within a unit cell

As one can see, the processes involve the accumulation, flow and cycling of materials ranging from water to decaying plant matter. The importance of material stocks and flows makes STELLA a natural software choice for representing the small scale dynamics of ecosystems. The software is also used to represent basic industrial disturbances that would link industrial mass flow models to ecosystem landscape models. The representation of these disturbances is a topic of later sections in Chapter 3.

3.1.3 Describing the Spatial Modeling Environment (SME)

   "The Spatial Modeling Environment (SME) is an integrated environment for high performance spatial modeling which transparently links icon-based modeling tools with advanced computing resources to support dynamic spatial modeling of complex systems" (Maxwell and Voinov 2004). Here, a modeling environment is defined as "an integrated set of software tools which provide the computer services necessary for simulation development and execution" (Maxwell 1999). The SME is based on a Modular Modeling Language (MML) that provides four general "computer services":

1. "…tools to import models from other languages into MSF [model specification formalism],"

2. "graphical tools to support MSF module development,"

3. "code generators to convert the MSF model specification into source code…"

4. "…extensive simulation services…" (Maxwell 1999).

Since the SME is a research project, not all of the computer services are robustly provided, but one can come to understand the SME by understanding these four services.

The SME takes a model "specification approach" to the development of a modular modeling architecture (Maxwell 1999). This approach requires the importation of models developed as modules to create a simulation. A specification approach is best understood in juxtaposition with the alternate "federated approach" to modular simulation creation. According to Maxwell, the federated approach "wraps" executables for many unassociated models to unite and form one large model - a computational hydra (Maxwell 1999). In contrast, the specification approach integrates models meant to be modules in a larger program (Maxwell 1999). These modules can conceivably exist in many different types of software languages; so, the SME includes a means of importing them. Currently, the SME can import models generated using STELLA. The STELLA models typically represent small scale ecosystem processes, as stated in Section 3.1.2. C++ models usually represent spatial (inter-unit cell) hydrology. The importing process generates a *.MML.* file that the user must configure; this importation configuration file links imported STELLA modules with the C++ models.

The SME currently out-sources the graphical module development service to STELLA. STELLA serves as the graphical module development tool. The previously

mentioned importation service converts STELLA module equations into a form that the SME can execute.

Once all necessary models have been imported into the MSF, the SME must convert the MSF into code for execution. The SME converts the MSF into C++ code using converters bundled with each SME distribution. Following conversion and compilation of the resulting C++ code, the user must configure another file; this second configuration file supplies the SME with parameters and links to files containing parameters. Once converted, compiled and configured, one possesses a spatially explicit, dynamic representation of an ecosystem.

The final group of computer services offered by the SME is grouped under the "extensive simulation services" heading. Though the documentation for the SME does not clearly state these services, one can estimate the extent of the services by working with the software and models implemented using the software. Storage and formatting for geographical information system (GIS) data are two critical computer services for which the system makes provisions. Ecosystem landscape models require significant amounts of GIS data; Table 3-3 lists some types of GIS data used in the PLM (Costanza, et al. 2002).

Table 3-3: Types of GIS Data Used in the PLM

Basic Types	Data Sets
Geographic	• Elevation • Watershed Boundary Data • Shoreline Delineation • Soil Type
Meteorological	• Ambient Temperature • Precipitation
Hydrological	• Ground Water Elevation • Bathymetry Data • Stream Flow • Surface and Ground Water Quality
Land Utilization	• Land Cover • Vegetation Index • Growth Coefficients

One uses GIS data to parameterize the individual STELLA modules, differentiate the unit cells on the spatial grid with respect to forcing function inputs (precipitation, wind, ambient temperature, etc.) and support the creation of multi-cellular structures such as rivers and streams. Spatial visualization is a second important service. The SME uses Java to create spatial maps for state variables in a particular ecosystem model. One views these maps at each time step, and when observed in sequence, they create time varying surfaces for selected state variables. One may see the data arrays used to create these surfaces using SME visualization tools. In principle, the visualization services also provide for the graphical representation of individual state variable values in selected cells versus time. Finally, the SME offers one uniform structure and repository for elements of the model ranging from configuration files to output data files.

3.2 Identifying Potential Links Between Ecosystem and Industrial Models

In the previous section, ecosystem landscape and industrial mass flow models were identified as the appropriate types of models to link to fulfill the requirements stated in Section 2.4.3. In Section 3.2, a decent into the details of linking the two types of models begins. The section identifies and justifies potential links between the two model types; by identifying links, this section completes the answer to thesis question 2a. Here, the task of forging links discussed in Section 3.3 is clarified by identifying the specific capabilities an eco-industrial model must possess.

3.2.1 Spatial Modifications

As noted in Sections 2.2.5 and 2.2.6, landscape models exist because of the importance of spatial positions and patterns in ecosystems. Voinov and coauthors allow for the modification of ecosystem patterns in their models (Voinov, et al. 1999a). The ability to modify these patterns and positions is industrially relevant for two reasons. First, facilities extract resources and release wastes at specific locations in the landscape. As a result of the spatially explicit structure of ecosystems, the same extractions and emissions can elicit different responses if they occur in different locations. Second, the placement of a facility can directly or indirectly change the habitat pattern in an ecosystem. The placement of a facility might significantly change the habitat of its site, or land uses around a facility might change to accommodate the new industry. The planting of crops for biomass based chemical processing and of trees for energy generation serve as examples (Galitsky, et al. 2003;Irving).

3.2.2 Time Varying Variables

The ability to vary facility inputs and output with time is an important capability. Demand for products changes; technology improves. New capacity is added, or old capacity is retired. These changes cause changes in facility extractions and emissions with time. Ecosystems also experience time varying inputs and outputs. Consequently, the Spatial Modeling Environment includes mechanisms that account for time dependent parameters (Maxwell 2002).

3.2.3 Mass Flow Modifications

As noted in Section 2.3.4, mass transfers in the form of extractions and emissions form one of the primary links between ecosystems and facilities. Water is often extracted from the environment for industrial processes. Sometimes this water evaporates and leaves the bounds of the industrial system, and sometimes it returns to the system. Biomass in the form of food and industrial crops is extracted from the system. Sections of forest are "clear-cut" to provide timber, pulp and paper or fuel. Agriculture introduces nutrients in the form of fertilizer and emits nutrients in the form of runoff. One can model water, biomass and nutrient mass transfers using the available ecosystem landscape modeling framework because it contains modules and / or C++ code that control the dynamics of each. One creates modules using STELLA software and adds C++ code within the SME. Costanza and coworkers have already modeled nutrient flows from anthropogenic sources such as farms and sewage facilities (Costanza, et al. 2002). Since the associated ecosystem responses have already been explored, this thesis focuses on industrial water and biomass flows.

3.2.4 Foreign Substances

A number of industrial pollutants are not commonly found in natural systems, and many of them cause profound environmental impacts. Unfortunately, the available ecosystem modeling framework lacks modules that represent the impacts and C++ code that describes the transport of these substances. Though the transport would require further development of the ecosystem modeling framework, one can potentially represent impacts by modifying ecosystem module parameters. Such an approach is not without precedent in environmental modeling. For example, DeAngelis and coauthors indirectly represent the impacts of contaminants by adjusting parameters and mechanisms in a Smallmouth Bass population model initially intended to represent populations in uncontaminated systems (DeAngelis, et al. 1991).

3.2.5 Controlling External Forcing Functions

Radiant energy and precipitation are major drivers of the ecosystem modeled by Costanza and coauthors (Costanza, et al. 2002). Temperature and wind also affect the system. These variables are exogenous, and they act as forcing functions for the ecosystem landscape model. Therefore, alterations in the long-term patterns of these variables influence the ecosystem. To understand an ecosystem's response to the combination of long-term forcing function dynamics and the presence of a facility, one must possess the ability to modify these forcing functions to simulate changes such as abnormal rainfall, extreme seasonal temperatures and other scenarios.

One can modify the time dependent data that supports these forcing functions, but the Hunting Creek model currently only allows runs of roughly 1.5 years. The 1.5 year limitation is caused by the current length of data arrays supporting the version of the

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Hunting Creek model used in this work. This short period of time does not allow the exploration of long-term dynamics. So, investigation of long-term dynamics and, therefore, the development of the capability to simulate the consequences of long-term industrial activity are considered beyond the scope of this thesis.

3.2.6 Summarizing Capabilities

Table 3-4 lists the industrially relevant capabilities identified in Sections 3.2.1 to 3.2.5. These are the capabilities the specific links must provide if an eco-industrial model is to harness the power of both ecosystem landscape and industrial mass flow models.

Table 3-4: List of Industrially Relevant Capabilities Offered by the Utilized Ecosystem Landscape Model (* Beyond the scope of this work)

#	Capability
1	Anthropogenic Input and Output Location Control
2	Landscape Modification
3	Time Dependent Variables
4	Water Mass Flow Control
5	Biomass Mass Flow Control
6	Nutrient Mass Flow Control*
7	Foreign Substances
8	Modification of External Forcing Functions*

Table 3-4 contains a starting point for creation of the links, the building blocks, needed to answer the second thesis question.

3.3 Creation of Linkages

In this section, six capabilities listed in Table 3-4 are transformed into building blocks for eco-industrial models. Starting with the capability to control space and concluding with the capability to represent the impacts of foreign substances, the section guides the reader through the set of modifications needed to interface industrial models with

ecosystem models. The section shows the reader how to represent links identified in Section 3.2 using the available tools selected in Section 3.1; the section answers thesis question 2b. In some cases, interfacing mandates modifications to the ecosystem models, and in others, existing ecosystem model features provide the necessary functions. In the former cases, the modifications are discussed, and their functionality is illustrated. For the later cases, the procedure for using the feature is outlined. The validity of the proposed industrial linkages to ecosystems is investigated in Chapter 4.

3.3.1 Controlling Location

The first capability listed in Table 3-4 is control of anthropogenic input and output location. Having created an industrially relevant material input or output (See Section 3.3.4), one follows four steps to establish control of its location.

1. Create a placeholder variable in the STELLA module to which the input or output applies, and link the placeholder to the input or output.
2. Configure the input or output to accept the placeholder as either a multiplying factor or a logical variable.
3. Create a "Study Area" sized map using a map format (PPM, M2, etc.) compatible with the Spatial Modeling Environment (SME).
4. Configure the <model_name>.conf file in the model's "Config" directory to accept the previously created map as the input for the placeholder variable.

Conceivably, one could also control location by developing custom C++ code, but the former method is used in this work.

One accomplishes the first two steps from within High Performance Systems Inc.'s STELLA software. Figure 3-4 illustrates the insertion of the placeholder called "Well Map."

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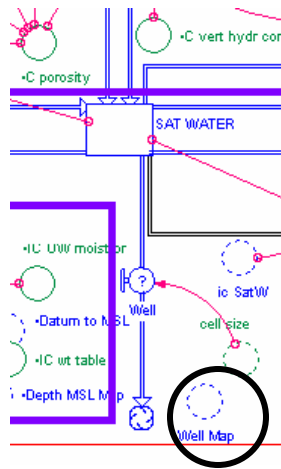
Figure 3-4: Creation of Placeholder "Well Map" for the Industrial Output "Well"
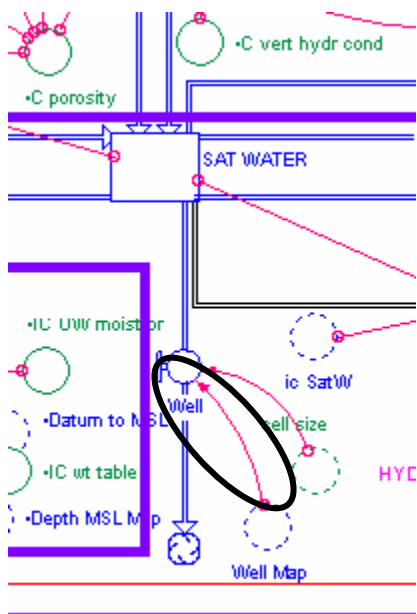
Figure 3-5: Linking the Placeholder
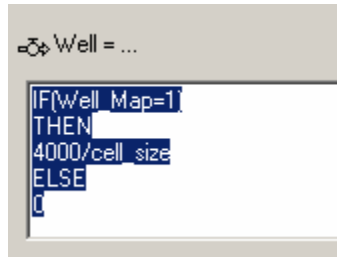
Figure 3-6: Configuring the Placeholder as a Logical Variable

Figure 3-5 demonstrates linking the placeholder with the anthropogenic output labeled "Well."   Figure 3-6 shows the configuration of the output, "Well," to accept the placeholder as a logical variable. If one configured the placeholder as a factor, one could control the location, but the control would be binary.

The second and third steps require the use of other software. Map creation requires the use of various geographical information system software packages (GIS) or text file editors. The simplest option is to use a text file editor to create a portable pixmap (PPM); Appendix A details the creation of SME compatible PPMs.   Preparation of the configuration file for the model occurs within the SME during model assembly.   The <model_name>.conf file contains a line for each variable in the model; so, for the discussed example, the file contains the variable named "Well Map." The text following the placeholder variable's name configures it as a spatial, time invariant variable:

* Well_Map d(P, GWater_Extract.ppm)

The configuration format is defined by Maxwell (Maxwell 2002). The position occupied by "P" indicates the type of map input to the SME, and "GWater_Extract.ppm" is the name of the file that contains this map.

After executing these steps, confirming the functionality of the spatial control involves running the model and visually inspecting two maps output by the SME. If

functional, the map for the placeholder variable should read zero except in the places specified as non-zero in the input map. Additionally, one should note change in the variable affected by the input or output centered near the non-zero locations. For example, "Well Map" is only non-zero in one cell, and groundwater experiences a significant drop in that cell (See Figure 3-7 and Figure 3-8).
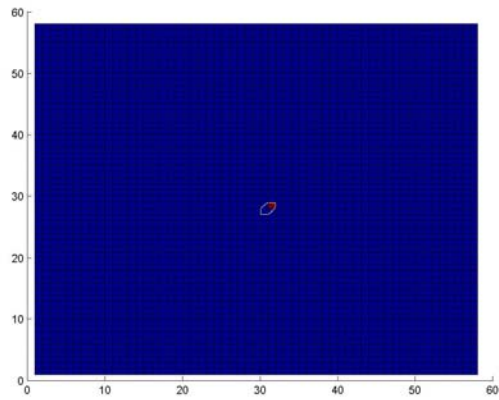
Figure 3-7: "Well Map" with One Active Cell at Position 30, 30
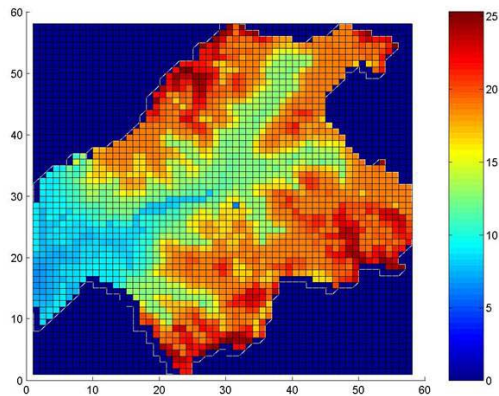
Figure 3-8: Ground Water Drop in the Vicinity of the Active Cell

3.3.2 Modifying the Landscape

The current ecosystem landscape model framework possesses the structures required to change landscape patterns. By modifying the appropriate class map in the "Data" directory of a model, one can change the habitat of a cell. Given the appropriate software, landscape modification should prove a straightforward task.

1. Open the class map using the appropriate software.
2. Change the desired landscape cells by editing elements of the array that represent different classes of land use. Each land use class is represented by an integer value; so, changing these integer values modifies the landscape.

Unfortunately, the current Hunting Creek landscape model uses M2 format maps to control landscape patterns. One cannot open or edit M2 using Linux or Windows software; so, the approach described above is only hypothetical. An alternative to this approach uses ArcInfo maps within the SME environment.

3.3.3 Variations with Time

Table 3-4 lists control of time dependent variables as the third capability. The SME contains data structures capable of handling time dependent variables; so, no modifications or additions are needed to implement time dependent industrial variables. One follows a three step procedure to create such variables.

1. Place a variable in the appropriate STELLA module.
2. Generate time series data for the variable, and place the data in a *.ts file. Maxwell recommends copying and modifying an existing *.ts file (Maxwell 2002).
3. Configure the time dependent variable in the <model_name>.conf file.

The configuration of a time dependent or "time series" variable uses the standard conventions for SME *.conf files (Maxwell 2002). For example, consider the variable "WELL_FLOW" found in the project "ChMort_WELLS."

* WELL_FLOWt(/usr/share/sme2/Projects/ChMort_WELLS/Data/wellflow.ts, 1)

The function "t(…)" defines the variable as a time series, and the directory "/usr/share…" indicates the location of the *.ts file "wellflow.ts." The number before the closing parenthesis declares the format of the *.ts file; format "1" is recommended.

3.3.4 Linking Mass Flows

Utilized ecosystem models allow consideration of three types of industrially relevant flows: water, nutrients and biomass. Implementing these flows is a matter of adding the appropriate terms to the appropriate module of the model in question. The appropriate term may depend upon the industrial situation.

Consider water usage and flows. Industrial models could potentially draw from ground and surface water stores in one or more cells in the ecosystem model. Simply adding an outflow variable to one of these stocks in the hydrology module creates a water extraction or input. In the case illustrated by Figure 3-9, "Well Out" is an extractive groundwater flow.
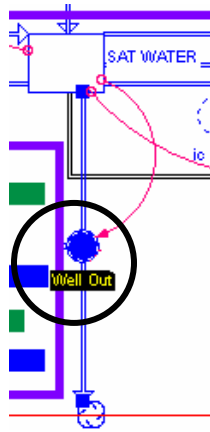
Figure 3-9: Addition of Anthropogenic Outflow "Well Out" to the Groundwater Stock

One parameterizes the magnitude of the water flow by adding a placeholder such as "Well Out Flow" (See Figure 3-10). As described in Section 3.3.1, one modifies the logic of the flow and adds another placeholder such as "g wmap" to control location.
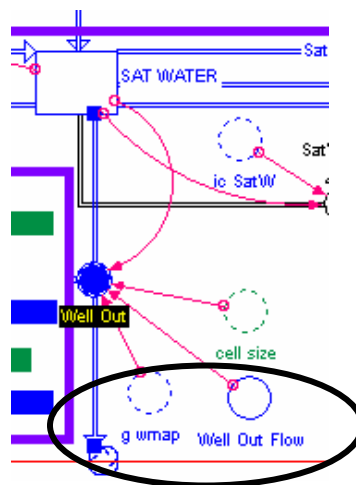
Figure 3-10: Addition of Placeholders for Magnitude and Position Control

A similar procedure describes nutrient loading, but the target of the operations is the nitrogen module. Inputs are added to the surface nitrogen stock labeled, "din_sf."

Biomass removal differs from the continuous and semi-continuous flows of water and nutrients in that three potential regimes exist: annual or less than annual harvesting, selective thinning and clear-cutting. Examples of industrial biomass harvesting include the harvest of corn for ethanol or chemicals production and the harvest of switch grass for

power production (Galitsky, et al. 2003;Mclaughlin, et al. 2002). Biomass removal in the

form of annual harvesting is already present, as the structure of the available macrophyte

module reveals (See Figure 3-11).
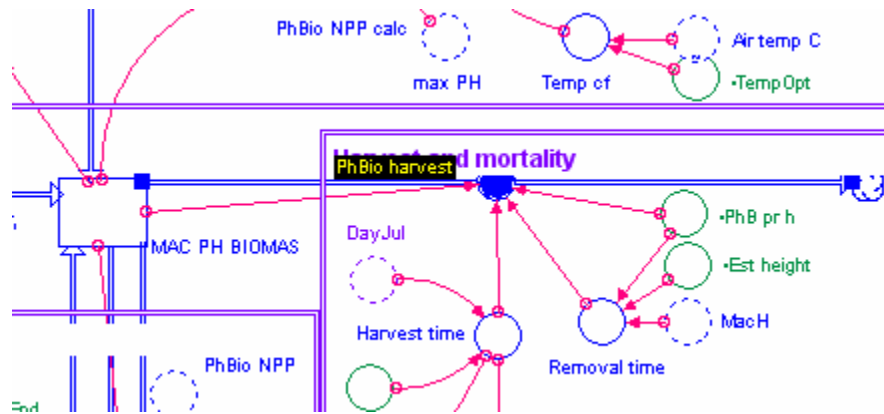
Figure 3-11: Harvest Variables in the Macrophyte Module (Voinov and Voinov 2003)

Selective thinning and clear cutting would apply to situations in which trees are felled for

timber, paper and power production. One uses the same procedure defined for water to

create these types of flows from the biomass stock.
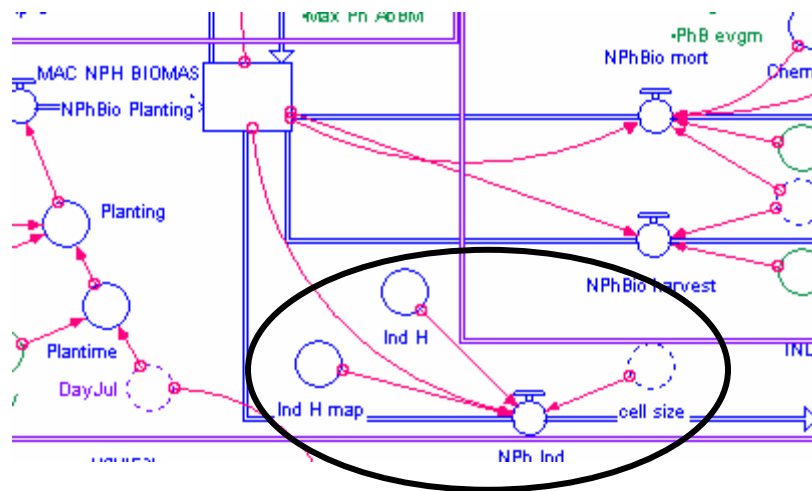
Figure 3-12: Variables and Parameters Needed to Allow Non-photosynthetic Biomass Removal

Figure 3-12   illustrates the use of flow ("NPH ind"), flow magnitude ("Ind H") and

map ("Ind H map") variables for biomass removals. High flow magnitudes would

represent selective thinning of forested cells while larger magnitudes would represent clear-cuts.

3.3.5 Representing the Impact of Foreign Substances

Representation of the impact of toxic materials requires an indirect approach. Modules for toxic materials are not available, but one can still represent impacts. As mentioned in Section 3.2.4, one can modify existing module mechanisms and change existing module parameters to account for these impacts. In this section, the non-photosynthetic biomass mortality mechanism in the macrophyte module is modified to represent the presence of a toxic substance. The net effect of the modification is an increase in the mortality rate for non-photosynthetic biomass.

One modifies the mortality mechanism by executing the outlined steps.

1. Create a placeholder variable in the Macrophyte STELLA module that represents the additional mortality fraction caused by the presence of a toxin.
2. Modify the non-photosynthetic mortality mechanism logic to incorporate the additional mortality fraction.
3. Create and configure a location control map as described in Section 3.3.1 to define the cells affected by the toxin.
4. Set the value of the mortality fraction in the <model_name>.conf file located in the model's "Config" directory.

In the macrophyte module, one needs to account for the magnitude and position of the toxin induced increase in mortality. The "Chem Mort" variable in Figure 3-13 is the placeholder for the mortality fraction, and the "Chem map" variable serves the same function for location.
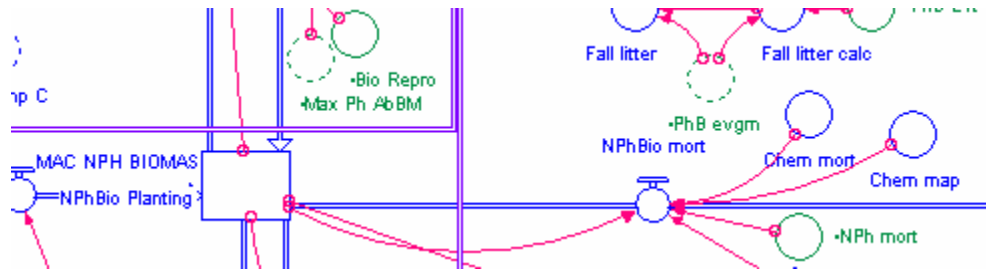
Figure 3-13: Non-photosynthetic Biomass Mortality Mechanism Modifications

The mortality mechanism logic in Figure 3-14 incorporates both of these additional variables. In this case, the total mortality fraction is assumed to be the sum of natural and toxic mortality.
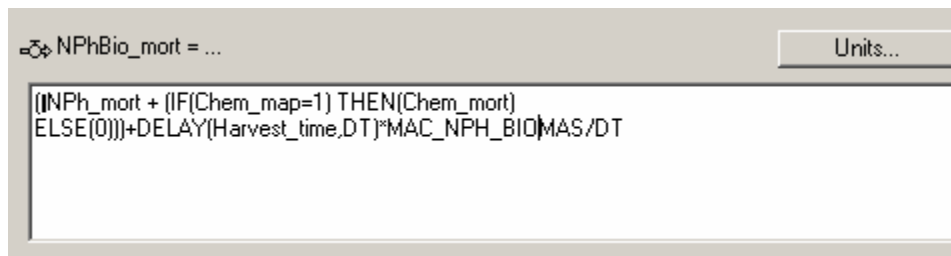
Figure 3-14: Mortality Mechanism Logic with Toxin Induced Mortality

Once the modified marcrophyte module is built into an ecosystem landscape model by the SME, one must set the value of the variable "Chem Mort" found in the model's <model_name>.conf file, as illustrated.

* CHEM_MORTpm(.0000535)

The "pm(…)" command simply defines the value of a SME model parameter (Maxwell 2002). The rationale behind selection of mortality fraction values appears in Section 4.7.2.

One may represent any substance that increases plant mortality in this manner, but the effects of such pollution would likely not be confined to a simple increase in mortality. The approach offers two advantages. First, it is simple, and second, it is general in the sense that one can represent any mortality increasing toxin. However, it is inaccurate

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because it does not include specific or general mechanisms through which various toxins act upon ecosystems. Germination and growth rates also change in the presence of toxins; these changes are not reflected in the current model. One could improve the approximation by including changes in these rates. Modifying the mortality fraction is, therefore, a crude, first-order approximation for the impact of toxic substances on ecosystems.

3.4 Connecting the Chapter with the Second Research Question

As discussed in Section 1.3.1, the second research question focuses on formalizing the links between models and on using existing tools to implement these formalized links. The previous sections first mapped requirements to existing models. The links needed to join the two existing model types were then identified in terms of capabilities. Finally, the sections converted the identified capabilities into concrete elements needed to link industrial models to ecosystem models. By using one or more of these elements, one can link an industry to an ecosystem. In Chapter 4, one finds an evaluation of the functionality of these links.

CHAPTER 4

Testing Eco-Industrial Model Linkages

In Chapter 4, the functionality of the linkages suggested and outlined in Sections 3.2 and 3.3 is tested and proved using the Hunting Creek ecosystem landscape model as an experimental apparatus. Besides demonstrating the effectiveness of the proposed linkage methods, the results of the simulation experiments yield an answer to the third thesis question. Observing the ecosystem model's response to the various anthropogenic manipulations reveals that one can detect ecosystem impacts using the discussed ecosystem landscape models.

4.1 Procedure for Testing the Functionality of Eco-Industrial Linkages

A procedure is needed to systematically test the functionality of the eco-industrial model linkages. This procedure must facilitate exploration of the response of the model to different types, intensities, locations and patterns of industrial disturbances. Each type of disturbance occurs at a number of locations, and at each location, the disturbance can occur at different intensities. These combinations suggest a hierarchical structure for the proposed experiments (See Figure 4-1). This section first gives an overview of the experiment procedure and structure, and then, subsections provide more detailed information concerning the elements of the structure.

As previously discussed, each linkage is embodied by a design variable. For a given response variable, a design variable may stimulate different responses for a given location and intensity. Changes in these design variables potentially cause changes in

multiple response variables. Figure 4-1 illustrates the relationship between design and response variables and the approach to investigating the influences of intensity and location.
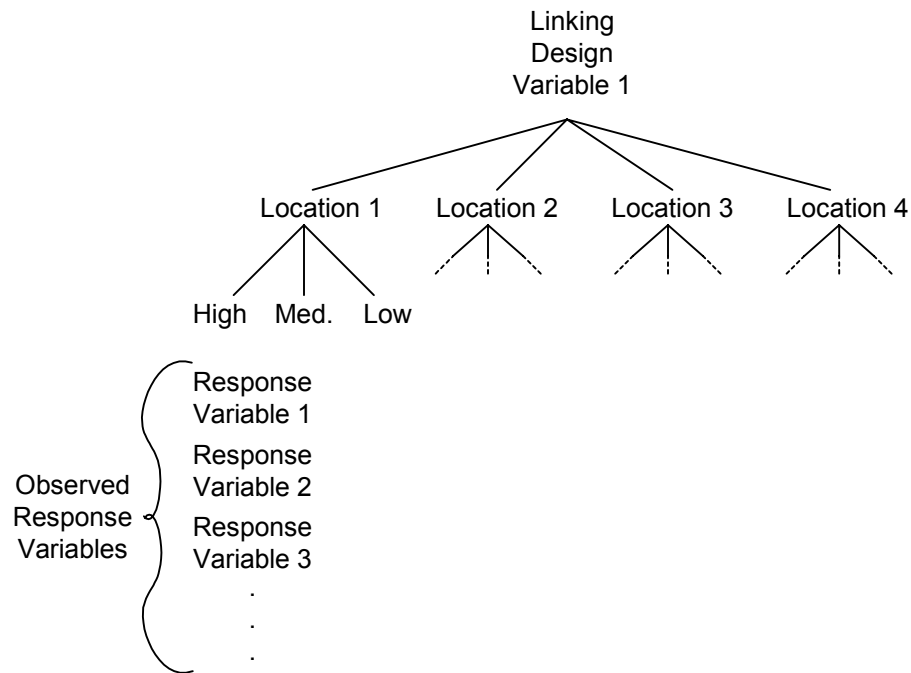
Figure 4-1: Structure for the Procedure

A design variable is applied at a number of locations, and at each location, its intensity is varied. For a given location and intensity, the response of the system is recorded for each observed response variable. For example, assume that groundwater extractions link industrial and ecosystem models; so, groundwater serves as the linking design variable. The groundwater extraction would be applied at four locations, and at each of the four, the rate of groundwater extraction would be set at one of three intensities. The impact of the groundwater disturbance at a given location for a given intensity would be observed by recording changes in a set of response variables such as groundwater amount, net primary production and others. Having observed the response to disturbances limited to

single cells, multi-cell disturbance patterns are then explored for selected combinations of design variables, intensities and patterns.

4.1.1 Design Variables

In the context of this thesis, the term, "design variable," possesses two definitions. A design variable is an aspect of the eco-industrial design controlled by the designer. It is also an element of the eco-industrial model varied to observe a response. Within the Hunting Creek watershed, the effect of six control (or design) variables on the ecosystem is explored (See Table 4-1). Humanity ostensibly controls these six design variables. The first four are linking design variables, and the last two are spatial design variables. Linking variables connect ecological and industrial systems using material flows while spatial variables account for the positions and patterns of the facilities extracting and releasing these materials.

Table 4-1: Design Variables

Design Variables	Description
Groundwater Flow	From pulp and paper production to beverage producers, many industries require water. This design variable represents the groundwater extractions required by industries.
Surface Water Flow	In some regions, hydrophilic industries have the option of drawing water from streams, rivers and lakes (i.e. surface water). This design variable exists to explore the consequences of extraction from these bodies of water.
Biomass Flow	A number of industries require biomass as a raw material. Pulp and paper production and some forms of power generation traditionally require biomass inputs. Potential chemical production systems also require biomass inputs (Galitsky, et al. 2003). The biomass design variable represents the continuous removal of biomass from the landscape to support such industrial activities.
Plant Mortality Fraction	Toxic industrial pollution causes ecosystem degradation. This variable crudely simulates degradation by increasing plant mortality.
Facility Location	Habitat, hydrology and other spatially variable factors influence the effects a facility causes in an ecosystem. So, different locations are explicitly considered in this experimental design for each of the preceding four linking design variables.
Industrialization Pattern	Habitat patterns influence ecosystem functions (Turner, et al. 2001). Patterns of industrialization may also influence ecosystem functions; so, the experimental design includes industrialization pattern as a design variable.

4.1.2 Response Variables

Changes in design variable flow intensities, positions or patterns elicit changes in the ecosystem model. One observes changes by recording the values of ecosystem model variables directly and indirectly affected by the design variables. One may call the affected variables "response variables" because they reveal the response of the ecosystem model to industrial disturbances. Table 4-2 lists and describes observed response variables.

<div align="center">**Table 4-2: Response Variables**</div>

Response Variables	Description
Net Primary Production (NPP)	NPP is the amount of organic matter added to plant tissues in a given amount of time (Odum 1987). It reveals the growth or decay of plants in an ecosystem.
Surface Nitrogen	The surface nitrogen variable represents the amount of nitrogen on the surface of a cell in Hunting Creek. One observes this variable because nitrogen influences plant growth and water quality (Schmitz 1996).
Groundwater	This variable is the amount of water in saturated underground storage. It responds directly to the groundwater flow design variable.
Surface Water	The surface water variable represents the amount of water stored on the surface in the form of streams, rivers, ponds and lakes. It directly responds to the surface water flow design variable.
Non-photosynthetic Biomass	Non-photosynthetic biomass represents the structural components of plants (i.e. trunk and branches of a tree). This variable responds directly to changes in biomass flow and plant mortality fraction.
Deposited Organic Material	Deposited organic material is dead plant matter in the process of decaying. Design variables that affect plant mortality indirectly affect the amount of decaying plant matter.

4.1.3 Selecting Design Variable Intensities

For each experiment, the influence of the design variable is explored at three different magnitudes. The magnitudes are characterized as high, medium and low. The values taken by these magnitudes relate to one or more industrial systems. For example, a high daily flow of biomass out of a forested cell would correspond to the daily consumption of wood biomass by a pulp and paper mill while a medium level flow would correspond to a moderately sized wood-fired power station. The types, sizes and relationships between the flows and industries depend upon the experiment in question, and therefore, they receive further treatment in the experiments.

4.1.4 Justifying the Selection of Disturbance Locations

Industrial disturbances are set to appear in four unique geographical locations in the Hunting Creek Watershed (See Figure 4-2). Table 4-3 contains the initial conditions for response variables at these locations. These positions were selected based upon their ability to affect nitrogen levels in the creek; initial model manipulations suggested the placements. It is expected that the disturbances will cause direct and indirect changes in NPP and that the changes will vary with location. The first location is north of the creek by 1400 m. Investigating disturbances in this region reveals their indirect relationship with nitrogen loading in the creek.

Table 4-3: Initial Conditions (1st day) for Primary and Experiment Specific Response Variables

Location	Groundwater [m]	Surface Water [m]	Surface Nitrogen [g/m2]	NPP [g/m2]	NPH Biomass [kg/m2]	Deposited Organic Material [kg/m2]
1 (25,15)	14.804	0	0.093553	0	46.040	1.0005
2 (30,30)	17.639	0	0.093675	0	46.040	1.0005
3 (35,50)	18.899	0	0.093731	0	46.040	1.0005
4 (32,18)	10.919	0	0.074047	0	0	1.0005
5 (32,19)	10.919	0	0.093712	0	46.040	1.0005
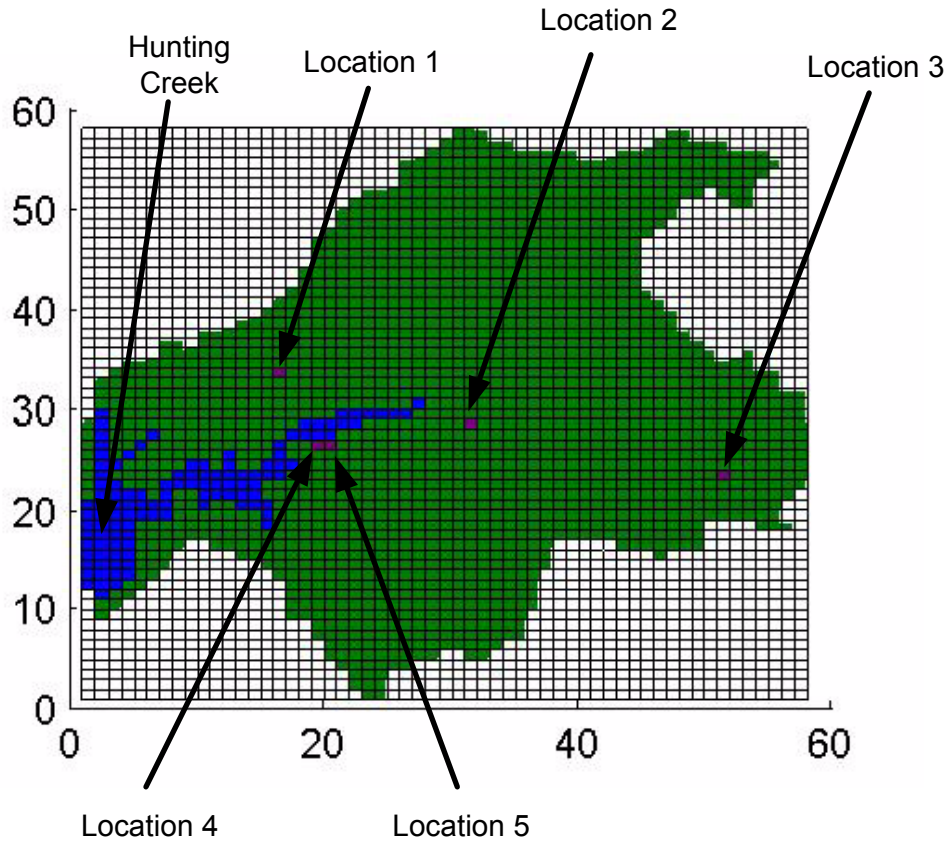
Figure 4-2: Locations of Disturbances in the Hunting Creek Watershed

The second location is the headwaters of the creek. Water and nutrients moving toward the creek from a large portion of the landscape congregate in the headwater area. Disturbances in the second location illuminate their amplifying or damping effect on nitrogen loading. Roughly 4100 m southeast of the headwaters, one finds the third location. Modifying this area shows the indirect effect of industry on the critical headwater region. Locations four and five fall south of and adjacent to the creek. Changes in this location reveal the direct effect of industrial activity on nitrogen loading in the creek.

4.1.5 Explaining the Size and Shape of Disturbances

In many of the experiments, the industrial disturbance occurs in one cell. However, the extent and pattern of industrial activity may play a role in determining the response of the ecosystem. The influence of landscape pattern on ecosystem function is already recognized in landscape ecology (Turner, et al. 2001). Different patterns of aggregately equivalent industrial activity may also elicit different ecosystem responses.

To explore the model's ability to investigate the effect of size and shape, one or more of three patterns are applied at selected locations (See Figure 4-3).
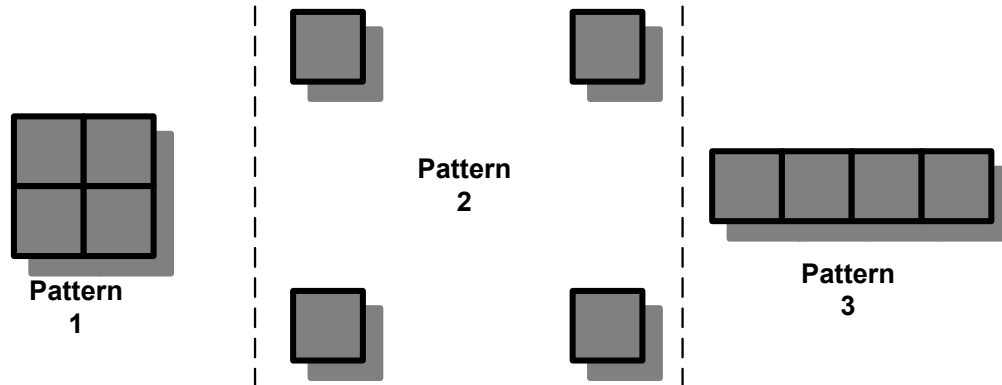
Figure 4-3: Multi-Cell Disturbance Patterns

The first pattern is a simple square block of cells; it is meant to represent the clustering of industrial activities. The second represents dispersion. The final, linear shape represents industrialization along a transportation corridor.

4.2 Hunting Creek as an Experimental Apparatus

The previous section described the procedure for investigating industrial disturbances, and it outlined the structure of the required experiments. To conduct experiments, one needs both a procedure and an apparatus – be it physical, mathematical or computational. Section 4.2 describes the apparatus that compliments the discussed procedure.

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4.2.1 Description of the Landscape and Model

Hunting Creek drains a small sub-watershed along the Patuxent River in southeastern Maryland. The area is dominated by forest and agricultural ecosystems, though some parts are in transition to other uses (See Figure 4-4).
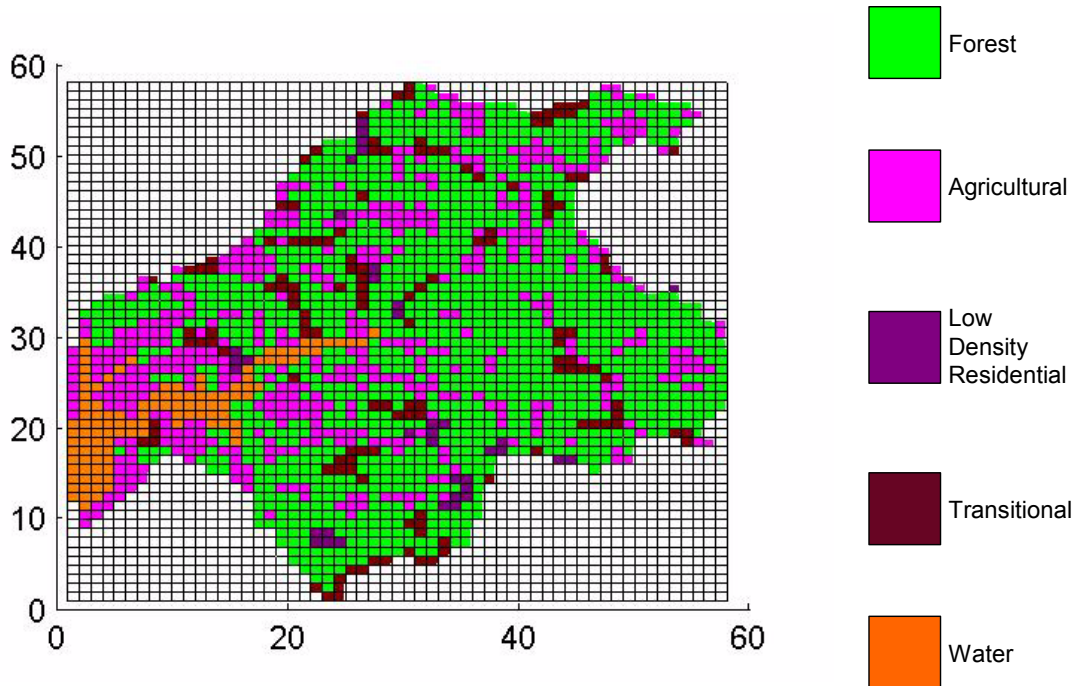
Figure 4-4: Land Use Map for Hunting Creek (40,000 m^2 cells)

Costanza and coworkers developed an ecosystem landscape model for the Hunting Creek subwatershed as part of PLM creation (Costanza, et al. 2002). The experiments outlined in the previous section use a version of the Hunting Creek model assembled from modules used to create the PLM. One can download these modules from the Library of Hydro-Ecological Ecological Models at the University of Vermont (Voinov and Voinov 2003). The modules encompass the ecosystem processes of unit cell hydrology, nutrient cycling, plant growth and decomposition. Modules for ecosystem parameters and global forcing functions, such as weather, are also used in the model. The SME developed by Maxwell and Costanza unites the modules within each cell and

connects each cell to form a spatially explicit watershed model (Maxwell and Costanza 1997).

4.2.2 Accuracy of Hunting Creek Model Outputs

Two sources indicate the accuracy of Hunting Creek Model outputs. Values reported in papers dealing with the Hunting Creek Model and the PLM potentially reveal the accuracy of the models. Statements by one of the model builders also cast light upon the accuracy of the models. Both information sources influence the presentation of results in Sections 4.3 through 4.7.

Table 4-4 contains the significant figures reported in the literature and suggested by Voinov for PLM and Hunting Creek Model outputs (Costanza, et al. 2002;Voinov 2004). In a personal communication, Voinov suggested that rounding to integers would be "safe" (Voinov 2004). So, one decimal place beyond the integer was selected as the uncertain figure for the third column in Table 4-4.

Table 4-4: Significant Figures for Response Variables

Response Variables	Least Significant Figure According to Papers	Least Significant Figure According to Modelers
Net Primary Production (NPP)	g	Tenth of a kg
Surface Nitrogen	mg	Tenth of a g
Groundwater	mm	Tenth of a m
Surface Water	mm	Tenth of a m
Non-photosynthetic Biomass	Tenth of a kg	Tenth of a kg
Deposited Organic Material	Tenth of a kg	Tenth of a kg

As one can see, the accuracy reported in the papers often exceeds the level of accuracy suggested by Voinov, and the number of figures output by the model would suggest even

greater accuracy than reported in the papers. Excess accuracy is likely presented in the papers to show the response of the models. The results presented in the following sections use the more conservative number of significant figures suggested by Voinov. Significant figures for the response variables appear in bold. The remaining digits appear in the tables as well; these "insignificant" figures are kept to illustrate model responses to disturbances. When reviewing the results, the reader must remember that one can only consider bold values detectable model responses.

4.2.3 Prior Uses

In the past, the Hunting Creek subwatershed model was used for calibration, the evaluation of land use experiments and landscape optimization. Costanza and coworkers initially created the 200 m cell model version to aid in calibration of the PLM (Costanza, et al. 2002). Run as part of the PLM at the coarser 1 km resolution, the Hunting Creek model contributed to achieving the goal of testing "…alternative scenarios of land use and patterns and management…" (Costanza, et al. 2002). The 200 m resolution model later found work as an analysis module for landscape optimization (Seppelt and Voinov 2002). The thrust of the effort centered upon demonstrating the usefulness of combining optimization with dynamic, spatially explicit ecosystem models to support agricultural land management decisions.

4.2.4 Hunting Creek and Eco-Industrial Modeling

In each experiment, one or more of the eco-industrial model building blocks identified and defined in Chapter 3 are added to the appropriate modules of the Hunting Creek ecosystem model. The building blocks embody the inputs, outputs and other

disturbances mandated by the procedure discussed in Section 4.1. Building and running models with these modified modules reveals the impacts of industrial disturbances upon the ecosystem. Table 4-5 lists experiments and sections where one may locate them.

Table 4-5: Experiments and Corresponding Sections in the Thesis

#	Experiment	Section	Numerical Results in Sections
1	Groundwater Disturbance	4.3	4.3.3 and 4.3.4
2	Surface Water Disturbance	4.4	4.3.3
3	Ground to Surface Water Disturbances	4.5	4.5.3 and 4.5.4
4	Gathering of Biomass for Industrial Use	4.6	4.6.3 and 4.6.4
5	Industrially Induced Macrophyte Mortality Disturbances	4.7	4.7.3 and 4.7.4

4.3 Experiment 1: Groundwater Extraction Disturbances

In the third chapter, water was identified as an industrial link that the available models could represent. This section tests one version of this anthropogenic mass flow link by exploring the industrial use of groundwater. It poses and checks hypotheses to assess the reasonableness of the representation. In this experiment, groundwater is assumed not to return to the Hunting Creek watershed.

4.3.1 Hypotheses

Groundwater extraction would hypothetically cause three noticeable changes.

1. First, groundwater level should drop in the vicinity of the extraction.

2. Second, surface water levels in the creek should fall because some precipitation infiltrates to replace a portion of the lost groundwater.

3. Finally, nitrogen concentration should rise in the creek as the amount of diluting water decreases.

To test these hypotheses, groundwater and surface water variables as well as the standard nitrogen and NPP are observed for simulations of groundwater extractions at various intensities.

4.3.2 Justifying Intensities of Groundwater Usage

For the four different locations, three intensities of ground water extraction are simulated. The values for these intensities correspond to amounts of water used by three different types of facilities. High intensity water extraction (37,800 m^3/day) corresponds to that of a pulp and paper mill while medium intensity (155 m^3/day) corresponds to a power plant with cooling towers (Cengel and Boles 1998). Low (16.5 m^3/day) corresponds to the water usage of a carpet manufacturing operation. One should note that the provided figure is not representative of carpet manufacturing operations that include dyeing.

4.3.3 Results: Single Disturbances

The spatially explicit ecosystem model allows observation of the geographic extent, pattern and magnitude of changes in the four response variables caused by groundwater extraction. Significant figures for these response variables appear in **bold** in the tables. Figure 4-5 illustrates the geographic extent and pattern of changes for the three extraction intensities on the 365th simulation day. The geographic extent of a change is associated with intensity. So, Figure 4-5 color-codes the extent changes according to intensity. Tables 4-6 to 4-10 contain values that indicate the magnitude of the changes. The names for the response variables are the same names that appear in the original Hunting Creek landscape model. SAT_WATER is the variable for groundwater; SURFACE_WATER is

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the variable for water on a cell's surface. DIN_SF represents nitrogen on the surface of a cell, and TOT_NPP stands for total net primary productivity or net primary production.

Tables 4-6 through 4-10 deserve some explanation. Table 4-6 contains response variable final states at four locations for the three disturbance intensities. The values in this type of table are absolute. If, for example, one wished to find the final groundwater level when a medium extraction is applied at the second location, one would read the value 11.812688 m from the fifth row in the third column. Table 4-7 contains the time, in days, required to initially exhaust the supply of groundwater in an extraction cell. "NA" appears for situations in which groundwater in a cell is not exhausted by the 365th day of the simulation. Table 4-8 also relates response variables, extraction intensities and locations, but the presented information differs in two important ways. First, the reported values are differences. The differences are obtained by comparing the disturbed landscape to an undisturbed baseline landscape. Mathematically, each response variable takes the form of an n x n matrix where n = 58 for Hunting Creek. If one identifies the undisturbed state variable (or baseline) matrix as **B** and the state variable matrix changed by an industrial disturbance as **C**, one finds the difference, **D,** using Equation 1.

$$D = C - B \qquad (1)$$

The values also differ because they represent sums of changes for all of the cells affected by a disturbance. In other words, each cell in Table 4-8 is the sum of the elements of a difference matrix created by disturbing the ecosystem with a given intensity at a given location (See Equation 2).

$$\text{Each Cell in Table 4-8} = \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} \qquad (2)$$

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To find the sum of the changes in surface water for high extraction at location 3, one would read the value -0.1827 m from the sixth row of the column marked "Location 3." Table 4-9 holds information about the extent of changes to the Hunting Creek watershed. Each cell in the table contains the number of cells in the Hunting Creek ecosystem landscape model affected by a given disturbance intensity at a given location. One finds this value, k, by counting the number of nonzero elements in the difference matrix, **D**. Table 4-10 contains values for a metric that is the quotient of the sum of the changes and number of cells affected. One calculates the metric by summing the elements of **D** and dividing by the number of nonzero elements, k, in the matrix to obtain an average difference for an area affected by a disturbance (See Equation 3).

$$metric = \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}}{k} \qquad (3)$$
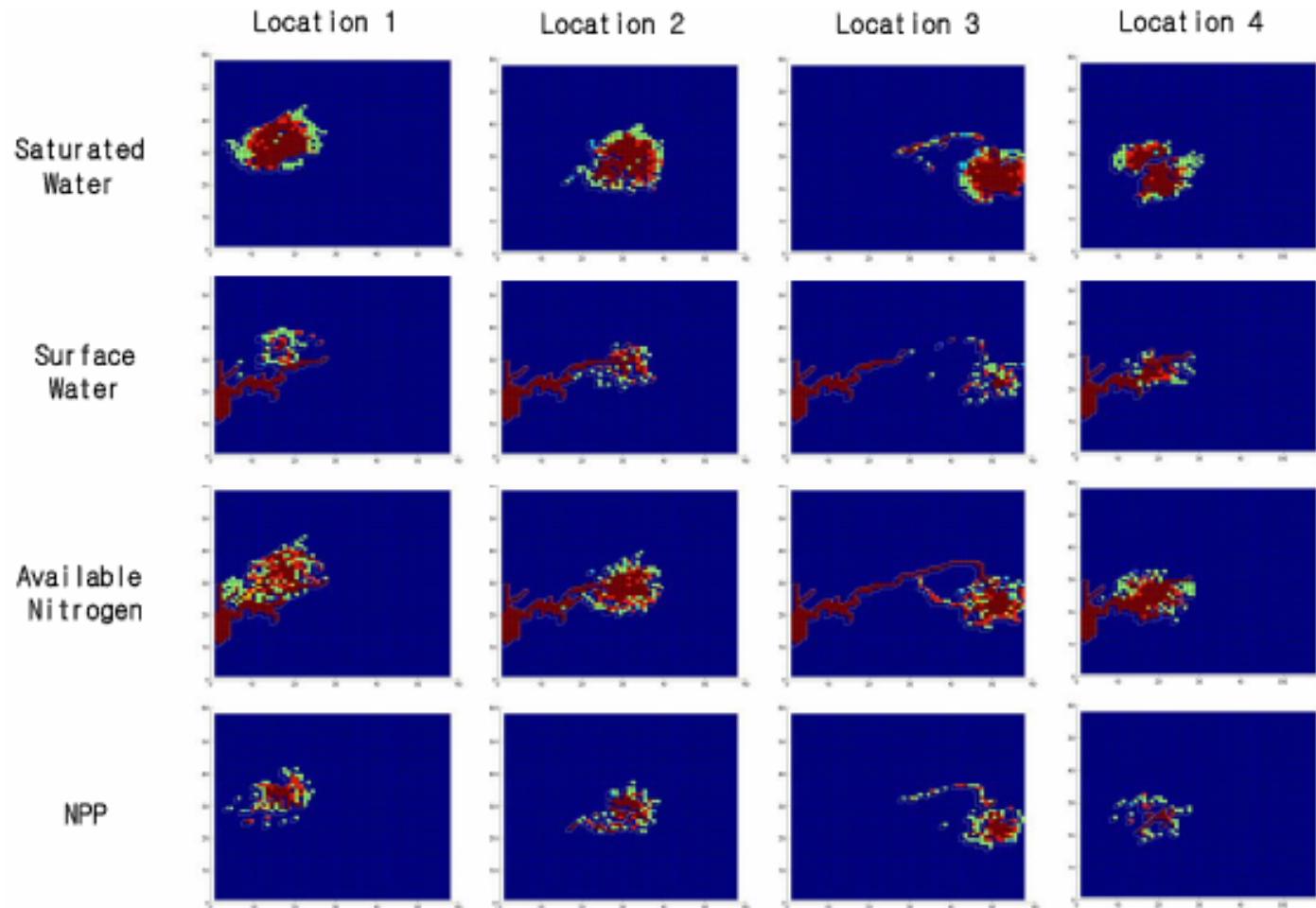
Figure 4-5: Extent and Pattern of Changes for Groundwater, Surface Water, Surface Nitrogen and Net Primary Production (NPP) at Different Hunting Creek Watershed Locations When Subject to a Groundwater Disturbance (Brown = all intensities; Pink = Med. And High; Green = High)

Table 4-6: Final State of Individual Cells Disturbed by Groundwater Extractions

Location	Water Extraction Intensity	Groundwater [m]	Surface Water [m]	Surface Nitrogen [g/m^2]	NPP [kg/m^2]
#1 (25,15)	Low	16.999577	0.002777	0.23238	3.516423
	Med.	16.400595	0.001269	0.051759	4.263627
	High	1.027508	0	0.055757	4.420037
#2 (30,30)	Low	13.842655	0	0.123733	4.346658
	Med.	11.812688	0	0.123856	4.354891
	High	0.868198	0	0.080664	4.136625
#3 (35,50)	Low	19.765408	0.00026	0.111469	4.431571
	Med.	17.055408	0	0.156677	4.472882
	High	0.654974	0	0.103646	4.488181
#4 (32,18)	Low	11.418938	0	0.053893	0
	Med.	8.795848	0	0.071638	0
	High	1.187473	0	0.054244	0

Table 4-7: Time to Initial Groundwater Exhaustion in Extraction Cell (days)

Intensity	Location 1	Location 2	Location 3	Location 4
Low	NA	NA	NA	NA
Med.	NA	NA	NA	NA
High	13	9	9	6

Table 4-8: Sum of the Changes for All Cells in the Area Affected by Groundwater Extractions

Response Variable	Water Extraction Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [m]	Low	-0.0512	-0.2648	-0.3975	-0.3976
	Med.	-1.2232	-2.9466	-4.0222	-3.6126
	High	-35.7362	-21.6806	-29.8735	-14.7325
SURFACE_WATER [m]	Low	-0.4391	-0.0275	-0.0248	-0.0179
	Med.	-1.3235	-0.241	-0.0594	-0.1699
	High	-3.3453	-1.8659	-0.1827	-1.1337
DIN_SF [g/m^2]	Low	-1.4253	-0.0813	0.0003	-0.0192
	Med.	-4.5946	-0.2457	-0.1789	-0.5441
	High	-11.2448	-3.3348	-0.3027	-1.8744
TOT_NPP [g/m^2]	Low	1050.7	8.7	8.9	-0.8
	Med.	1789.1	46.9	9.2	-25
	High	3852.1	-167.8	23.9	39.7

Table 4-9: Number of Cells Affected by Groundwater Extractions for the Stated Intensities

Response Variable	Water Extraction Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [affected cells]	Low	128	129	133	121
	Med.	157	162	180	140
	High	237	232	216	192
SURFACE_WATER [affected cells]	Low	120	146	133	133
	Med.	139	160	147	146
	High	177	187	186	166
DIN_SF [affected cells]	Low	196	206	219	183
	Med.	230	236	263	199
	High	321	288	298	243
TOT_NPP [affected cells]	Low	44	49	39	20
	Med.	60	67	65	28
	High	108	102	122	56

Table 4-10: Average Change for a Response Variable in an Area Affected by a Groundwater Disturbance for the Stated Intensities

Response Variable	Water Extraction Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [m / affected cell]	Low	-0.0004	-0.0021	-0.003	-0.0033
	Med.	-0.0078	-0.0182	-0.0223	-0.0258
	High	-0.1508	-0.0935	-0.1383	-0.0767
SURFACE_WATER [m / affected cell]	Low	-0.0037	-0.0002	-0.0001861	-0.0001
	Med.	-0.0095	-0.0015	-0.0004038	-0.0012
	High	-0.0189	-0.01	-0.0009825	-0.0068
DIN_SF [g/m^2*affected cell]	Low	-0.0073	-0.0004	0	-0.0001
	Med.	-0.02	-0.001	-0.0007	-0.0027
	High	-0.035	-0.0116	-0.001	-0.0077
TOT_NPP [g/m^2*affected cell]	Low	23.9	0.2	0.2288	-0.0407
	Med.	29.8	0.7	0.1423	-0.8915
	High	35.7	-1.6	0.1956	0.7093

4.3.4 Results: Different Disturbance Sizes and Shapes

Three patterns described in Section 4.1.5 are applied to the first location with a cumulative intensity equivalent to that of one high intensity disturbance. So, the high intensity water extraction value is divided among four cells for the square, line and distributed patterns. These patterns could represent one facility drawing resources from multiple locations, or depending upon the industry, they could represent multiple smaller facilities taking the place of one larger one. Response variable values are contained in

Table 4-11 through Table 4-13. These tables present data meant to shed light upon the influence of industrial disturbance patterns on the modeled ecosystem.

Table 4-11: Sum of Magnitudes for Patterns of High Intensity Extraction at Location 1

Pattern	Response Variables			
	SAT_WATER [m]	SURFACE_WATER [m]	DIN_SF [g/m^2]	TOT_NPP [kg/m^2]
Square	**-117.3**711	**-6.1**684	**-17.5**008	**4.6**988
Line	**-106.1**688	**-3.6**518	**-11.7**059	**3.9**811
Distributed	**-115.9**545	**-6.7**959	**-18.1**503	**4.1**205

Table 4-12: Number of Cells Affected by High Intensity Extraction at Location 1

Pattern	Response Variables			
	SAT_WATER [affected cells]	SURFACE_WATER [affected cell]	DIN_SF affected cell]	TOT_NPP [affected cell]
Square	252	188	333	119
Line	244	189	322	115
Distributed	257	193	336	118

Table 4-13: Average Change for Response Variables Affected by High Intensity Extraction at Location 1

Pattern	Response Variables			
	SAT_WATER [m]	SURFACE_WATER [m / affected cell]	DIN_SF [g/m2*affected cell]	TOT_NPP [kg/m2*affected cell]
Square	-0.4658	-0.0328	-0.0526	0.0395
Line	-0.4351	-0.0193	-0.0364	0.0346
Distributed	-0.4512	-0.0352	-0.054	0.0349

4.3.5 Discussion of Results

In this section, observed changes in response variable values for groundwater, surface water, surface nitrogen and NPP are compared with changes hypothesized in Section 4.3.1.   Responses corresponding with expectations are first discussed, and then, unexpected system responses are considered. The influences of location and pattern are also noted.

For each response variable at the four locations, two hypothesized patterns are common.   Changes center upon the point of groundwater extraction, and higher

extraction intensities affect larger areas of the watershed. In each panel of Figure 4-5, one clearly sees that differences at all three intensities cluster around the extraction locations. Higher extraction intensities affect progressively more cells, as made evident by the higher bars in Figure 4-6. Table 4-9 contains the same information in numerical form. Taking the geographic extent of saturated water changes at the first location as an example, one notes that low intensity groundwater extraction affects 128 cells, medium intensity affects 157 and the highest intensity extraction affects 237.
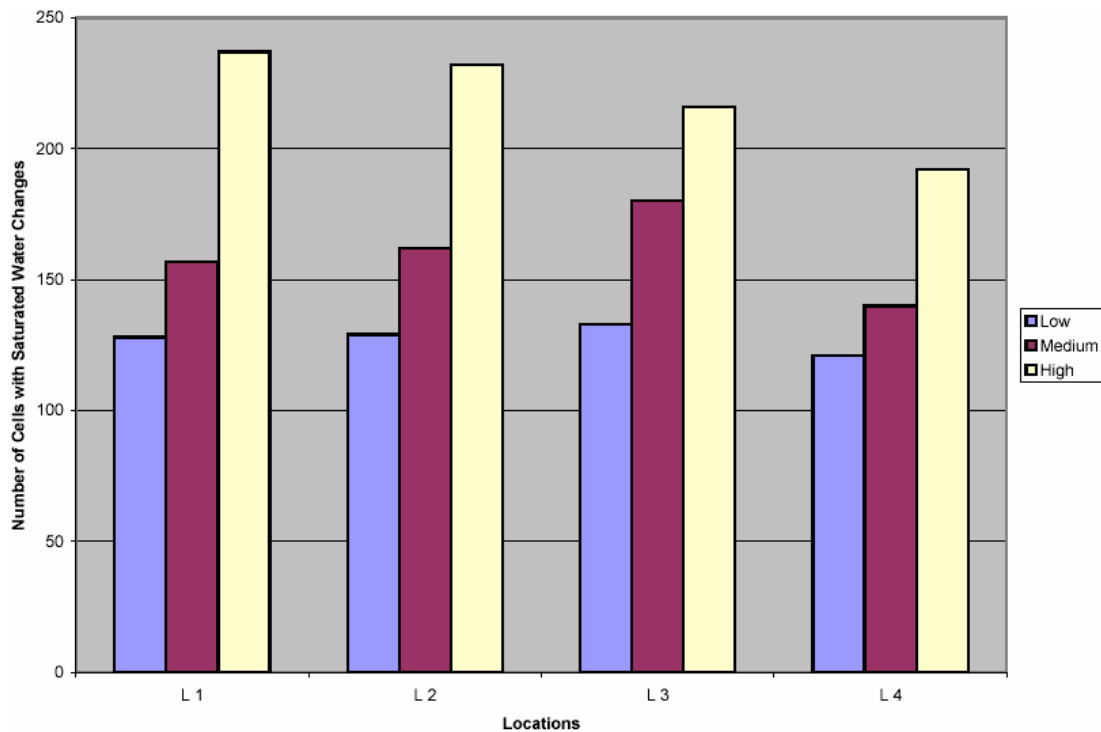
Figure 4-6: Number of Cells with Saturated Water Changes at Three Intensities vs. Location

As expected, groundwater in the vicinity of the extraction drops. This drop leads to a reduction in creek surface water, and in areas that temporarily accumulate surface water as a result of precipitation events, surface water also drops. All three multi-cell patterns show more precipitous declines in saturated and surface water (See Table 4-11 and Table 4-13). The highest total saturated water change is -117.4 m for the square pattern as

compared to a change of -35.7 m for a single cell disturbance of the same intensity at the same location. The higher water removal for patterns results from the fact that at high intensity single cells cease yielding water before the simulation ends. Since patterns divide the same intensity over multiple cells, water extraction continues for a longer period of time. One should note that the subsurface hydrology model does not appear to have been designed to accurately represent groundwater exhaustion. It is likely that pumping cells down to nearly zero saturated water produces quantitatively inaccurate results. In fact, the hydrology module needed some minor modifications to prevent negative groundwater levels during extraction! A surface plot reveals that the primary surface water declines occur in the creek (See Figure 4-7). Surrounding cells experience far smaller declines. *Taken together, these findings support the first two hypotheses stated in Section 4.3.1. Specifically, groundwater in the vicinity of an extraction drops, and creek surface water also declines.*
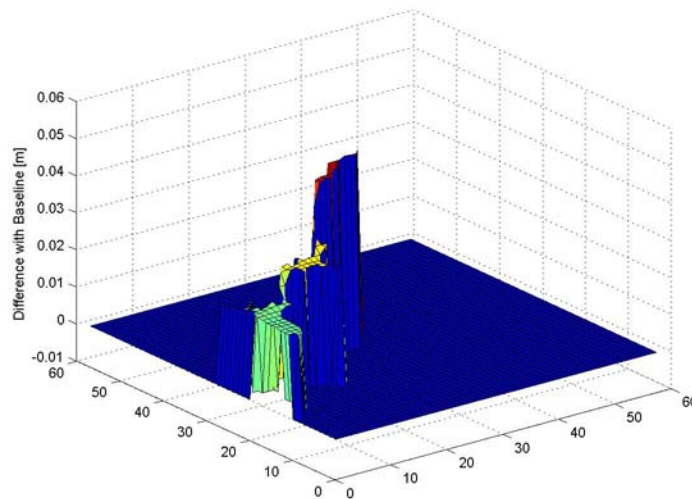
Figure 4-7: Surface Representing Difference in Surface Water Height for Location 1 subject to High Extraction Intensity (negative values made positive for clarity)

Interestingly, more than one mechanism may link surface water drops with groundwater extractions. Groundwater exhibits interesting behavior in the fourth location. Levels beneath the creek do not change, but groundwater levels on the bank opposite the withdrawal point do change. The decline in saturated water levels may allow greater absorption of surface water, which in turn prevents water from reaching the creek, but the saturated water pattern in the fourth location at least suggests an additional mechanism (See Figure 4-5). The creek cuts through the heart of the disturbed saturated water region in location four. In cells containing the creek, saturated water does not experience a decline, despite proximity to the extraction epicenter. Since the creek's surface water and the saturated water zone remain in contact for the entire simulation period, the creek appears to be compensating for saturated water losses. Water from the creek is passing directly into saturated storage instead of first infiltrating through an unsaturated layer of soil; surface water in the creek is directly compensating for saturated water losses. According to the designers of the model, "all surface water is removed by horizontal runoff or by replenishing the saturated water in case that storage has been drained" (Voinov, et al. 1999b). So, direct compensation is another mechanism that allows surface water levels to decline.

The decline in surface water levels was hypothesized to herald an increase in creek nitrogen concentrations. However, as Table 4-10 shows, average nitrogen declines exceeded surface water drops with the result that nitrogen concentration decreased. In the first location for both single cell and pattern disturbances, one may partially attribute the nitrogen losses to significant increases in NPP. The reasons behind the net loss of nitrogen in other locations are not clear. Despite having less surface water to mobilize

nitrogen and less primary production to consume nitrogen, surface nitrogen levels decline at location 2 when a disturbance is introduced. For example, surface nitrogen levels listed in Table 4-8 decline by 3.33 g/m^2 despite the fact that NPP falls by 167.8 g/m^2. One would expect a negative correlation between these response variables. More NPP should require more nutrients; less NPP should require fewer nutrients. The third and fourth locations exhibit similar unclear behavior. This result demonstrates the potential pitfalls of allowing even informed intuition to estimate the response of a complex, nonlinear system.

Surprisingly, groundwater reductions affect total net primary productivity (NPP). For groundwater, surface water and nutrients, the magnitudes of the changes increase with extraction amount, but this trend does not hold for total net primary productivity in locations 2-4 (See Figure 4-8).
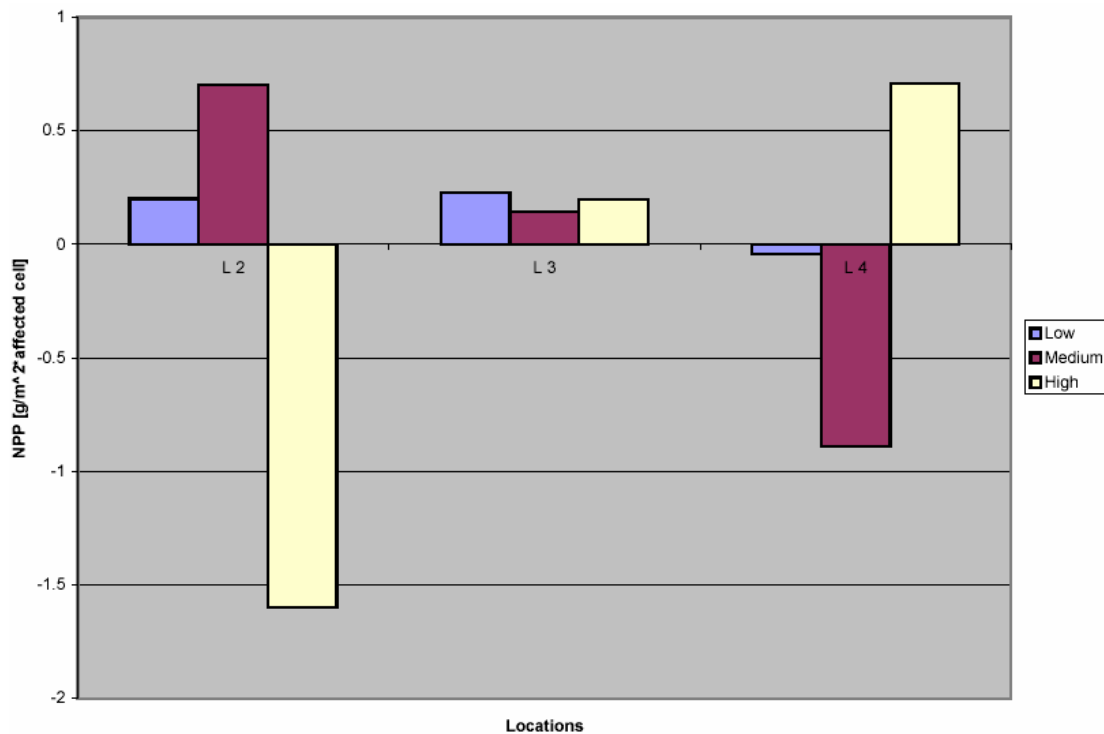
Figure 4-8: Average NPP Change per Cell at Three Intensities vs. Locations 2-4

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Increasing groundwater extraction increases net primary production in the first location by as much as 37.5 g/m^2*affected cell, but as the third bar in Figure 4-8 indicates, the highest intensity causes a net primary production decrease at location two. Net primary production in location three benefits from extraction, but the benefits do not correlate with extraction intensity. Oddly, the fourth location exhibits a trend opposite to that in the second location. Low and medium intensity extractions cause NPP decreases while high intensity groundwater usage leads to a NPP increase.

"Geography matters." Despite experiencing the same disturbances, each location manifests different response patterns and magnitudes (See Figure 4-5 and Table 4-10). In the case of net primary production, trends even reverse in different locations. The contradictory NPP trends may stem from an interaction among surface nitrogen, surface water and habitat type. Disturbance patterns appear less influential than location. Besides the previously explained difference in water extraction magnitudes, the three different multi-cell disturbance patterns applied at the first location caused ecosystem responses similar to those precipitated by the single-cell disturbance.

Finally, plotting the change in groundwater level as a surface may have uncovered a limitation in the model's ability to represent sub-surface hydrology. Plotting the difference in saturated water height between the baseline and the high intensity water extraction experiment at the first location reveals that the greatest change occurs in the extraction cell (See Figure 4-9).
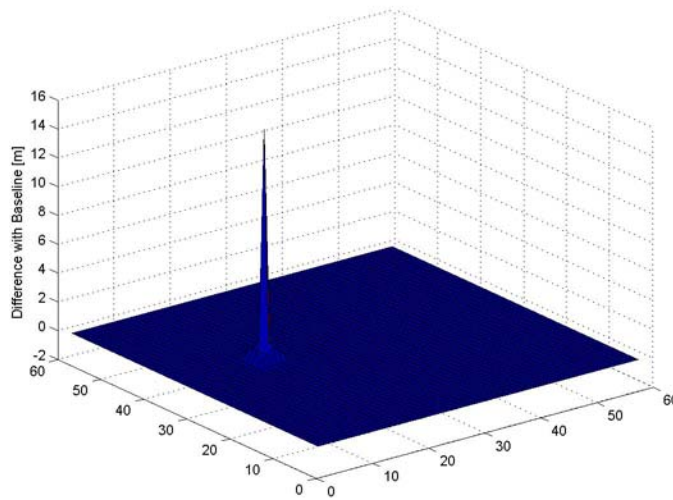
Figure 4-9: Surface Representing Difference in Saturated Water Height for Location 1 subject to High Extraction Intensity (negative value made positive for clarity)

While one would expect high losses at the point of extraction, the spike in Figure 4-9 may not accurately represent the physics of the situation. Comparing Table 4-6 with Table 4-8, one notes that the model predicts ~50% or more of the removed groundwater originates in the extraction cell; adjacent cells experience losses more than an order of magnitude less than the extraction cell. Perhaps, this type of phenomenon requires a finer spatial resolution, or perhaps, the model's sub-surface hydrology algorithm or water extraction algorithm need modification to function in the intended capacity.

The results of extracting groundwater from the Hunting Creek watershed begin to reveal the complex interactions between ecosystem processes, and they underscore the sometimes counter-intuitive responses of ecosystems to disturbances. Hypotheses concerning the ground and surface water responses gain support from the results while the hypothesis concerning surface nitrogen is called into question. The response of the system at multiple intensities and the presence of trends provide partial answers to thesis questions 3a and 3b respectively. The reasonableness of the ground and surface water

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responses supports an affirmative answer to question 3c. The importance of location is confirmed. On a related, practical note, the exhaustion of groundwater as a result of industrial activity underscores the importance of scaling a facility to fit the physical constraints of its surroundings. Different multi-cell patterns cause behaviors similar to their single disturbance counterparts. And, the results may highlight some model limitations, providing part of the answer to question 3d.

4.4 Experiment 2: Surface Water Extraction Disturbances

This section continues the investigation of anthropogenic water disturbances started in Section 4.3. Surface water is removed from the system at two different points (pt. A [31, 16] and pt. B [37, 3]) along Hunting Creek's watercourse. At each extraction point, the simulation is run for three different water usage intensities. Surface water is assumed not to return to the system as a result of evaporation or incorporation into products. Hypotheses advanced in Section 4.4.1 are checked in Section 4.4.4 to assess the reasonableness of the representation.

4.4.1 Hypotheses

Here, five hypothesizes concerning the response of the ecosystem are forwarded. These hypothesizes focus the discussion of results in Section 4.3.5.

1. For each surface water withdrawal intensity, one would expect to see a decline in the overall volume of water in the creek

2. The amount of the decline should positively correlate with the intensity of the withdrawal.

3. Since surface water mobilizes nitrogen, a drop in surface water should lead to an accumulation of nitrogen in the creek.

4. Terrestrial nitrogen amounts should not change.

5. Given the large volume of water in the creek, the planned extractions should not impact saturated water levels or net primary production.

4.4.2 Justifying Intensities of Surface Water Usage

Once again, pulp and paper, power generation and carpet manufacturing provide the high, medium and low water usage intensities. Industries and communities often draw water from both ground and surface sources. Therefore, it is reasonable to use the same intensities applied to groundwater. Furthermore, using the same intensities allows comparison among experiments.

4.4.3 Results: Single Disturbances

In a manner similar to Section 4.3, Figure 4-10 illustrates the geographic extent and pattern of changes for the three extraction intensities on the 365th simulation day. Table 4-14 contains values that indicate the magnitude of the changes. Table 4-15 numerically indicates the extent of the changes, and Table 4-16 combines magnitude and extent to provide an indicator for the average change in each cell of the landscape. Significant figures for response variables appear in **bold** in the tables.
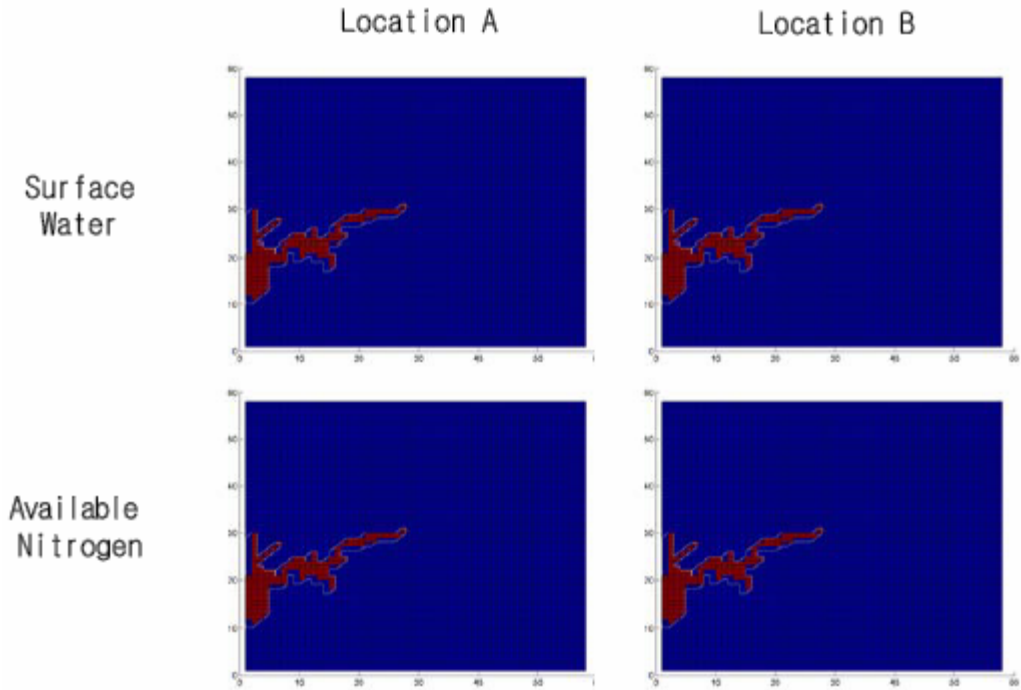
Figure 4-10: Geographic Extent and Pattern of Changes for Surface Water and Surface Nitrogen at Two Different Locations in the Hunting Creek Watershed When Subject to a Surface Water Disturbance

Table 4-14: Sum of the Changes for All Cells in the Area Affected by Groundwater Extractions

Variable	Intensity	Location A	Location B
SURFACE_WATER [m]	Low	**-0.1**485	**-0.1**399
	Med.	**-1.3**951	**-1.3**145
	High	**-48.7**1	**-6.8**128
DIN_SF [g/m^2]	Low	**-0.0**006	**0.0**029
	Med.	**-0.0**049	**0.0**262
	High	**-0.2**325	**0.5**812

Table 4-15: Number of Cells Affected by Groundwater Extractions for the Stated Intensities

Variable	Intensity	Location A	Location B
SURFACE_WATER [affected cells]	Low	113	113
	Med.	113	113
	High	113	113
DIN_SF [affected cells]	Low	113	113
	Med.	113	113
	High	113	113

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Table 4-16: Average Magnitude of Change for a Response Variable in an Area Affected by a Surface Water Disturbance

Variable	Intensity	Location A	Location B
SURFACE_WATER [m / affected cell]	Low	-0.0013	-0.0012
	Med.	-0.0123	-0.0116
	High	-0.4311	-0.0603
DIN_SF [g/m2*affected cell]	Low	0	0
	Med.	0	0.0002
	High	-0.0021	0.0051

4.4.4 Discussion of Results

In what follows, the ecosystem impacts as characterized by the observed response variables are discussed. Response variable behavior is compared with the behavior hypothesized in Section 4.5.1. Results supporting and refuting the hypotheses are discussed.

Figure 4-10 reveals that changes in surface water level and nitrogen amounts are confined to the area occupied by Hunting Creek. Maps for saturated water and net primary production are absent because these variables did not change in response to surface water extractions. *Surface water levels dropped in correspondence with extraction intensity, which supports the first two hypotheses* (See Table 4-14 and Table 4-16). For example, Table 4-14 shows that sum of surface water changes at Location A ranged from -0.15 m for low intensity through -1.40 m at medium to -48.71 m for high intensity surface water extraction. *An absence of changes in saturated water, NPP and terrestrial nitrogen levels lends support to the fourth and fifth hypotheses in Section 4.4.1.*

Nitrogen trends do not support the hypothesis that reducing surface water allows nitrogen accumulation. Interestingly, the extraction location caused changes in creek nitrogen levels. Removing water in the upstream location, Location A, caused a drop in overall nitrogen levels, but removing water downstream at Location B caused an increase in surface nitrogen levels. At Location A, nitrogen differences ranged from -0.0006 g/m^2

at low intensity to -0.2325 g/m^2 at high intensity, but at Location B, the differences ranged from 0.0029 g/m^2 to 0.5812 g/m^2. Results for the downstream site support the hypothesis, but upstream site results show a decrease in nitrogen despite a decrease in surface water. Despite the overall negative value of the average magnitude, extracting water from Location A does increase the amount of nitrogen that accumulates at the outlet of Hunting Creek.

Once again, one sees evidence that the system responds to reasonable industrial changes, which lends credibility to a positive answer to thesis question 3a. With the exception of surface nitrogen, the simulation results support the hypotheses stated in Section 4.4.1. Surface water decreases; the magnitude of the decrease correlates with intensity increases. These trends constitute part of the answer to question 3b, and the reasonableness of the system response strengthens the argument for an affirmative answer to question 3c. Changes in the creek do not affect terrestrial nitrogen amounts, as one would expect. The creek does not empty at the considered intensities; so, groundwater levels are not disturbed. Since surface water and nitrogen changes are indeed confined to the creek, the results show the expected lack of change in NPP.

4.5 Experiment 3: Ground to Surface Water Disturbances

In this final section dealing with water disturbances, two different types of disturbances are simultaneously applied to the watershed, and the resulting effects are observed. Groundwater is transferred from the saturated water zone and released on the surface at four different locations. Some basic hypotheses are posed and checked, but the experiment primarily exists to explore the response of the system to more complicated stimuli.

4.5.1 Hypotheses

In the third experiment, five hypothesized ecosystem model responses are likely. The hypothesized responses include changes in variables directly and indirectly affected by groundwater extraction and surface release.

1. As with the groundwater extraction experiment, one would expect saturated water levels to fall as groundwater is transferred to the surface.

2. One would expect water to accumulate on the surface, though accumulation would be balanced by infiltration to the unsaturated layer.

3. One would also hypothesize changes in surface nitrogen patterns as a result of mobilization by surface water accumulating and moving toward Hunting Creek. Nitrogen pattern changes would likely correspond with changes in runoff.

4. NPP differences would also appear. Nitrogen and water influence NPP; so, differences in NPP patterns would in part depend on surface water and nitrogen.

5. It is likely that NPP would decrease at the point of surface water release because of increased macrophyte mortality.

4.5.2 Justifying Intensities of Groundwater Extractions and Surface Water Releases

This experiment is somewhat artificial in that groundwater removed at an industrial site rarely exits the industrial system as surface water at the same site. The primary purpose of the experiment is to explore the collocated disturbances of groundwater extraction and surface release. Given the artificial nature of the experiment, intensities remain at the same three levels used in the previous two experiments for reasons of consistency and comparability.

4.5.3 Results: Single Disturbances

This section contains graphical and numerical results of transferring groundwater to the surface for three different intensities at four different locations. The data formats are identical to those already encountered, and as in the previous sections, significant figures for response variables appear in **bold** in the tables.
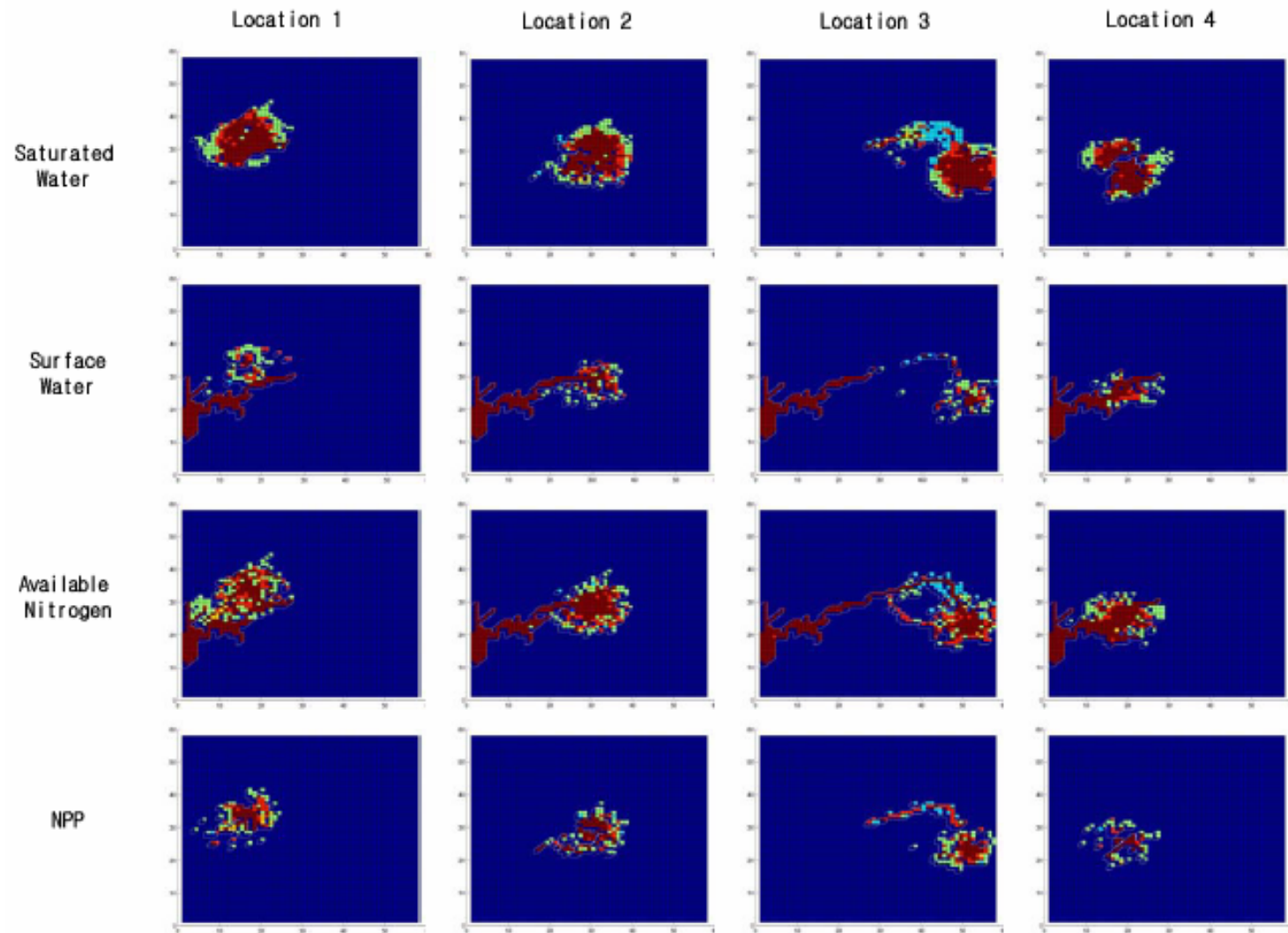
Figure 4-11: Geographic Extent and Pattern of Changes for Groundwater, Surface Water, Surface Nitrogen and Net Primary Production (NPP) at Four Different Locations in the Hunting Creek Watershed When Subject to a Groundwater Extraction and Surface Release Disturbance

Table 4-17: Final State of Individual Cells Disturbed by Different Intensities of Ground to Surface Water Transfers

Location	Water Extraction Intensity	Groundwater [m]	Surface Water [m]	Surface Nitrogen [g/m²]	NPP [kg/m²]
#1 (25,15)	Low	16.999577	0.00319	0.232378	3.515038
	Med.	16.399378	0.005144	0.051759	4.262791
	High	1.027626	0	0.055749	4.412816
#2 (30,30)	Low	13.851686	0.000412	0.08896	4.231412
	Med.	11.815125	0.003875	0.088946	4.240788
	High	0.868222	0	0.080613	4.134002
#3 (35,50)	Low	19.787798	0.000676	0.111542	4.407678
	Med.	17.057976	0.003874	0.112117	4.40784
	High	0.654979	0	0.10352	4.484857
#4 (32,18)	Low	11.418938	0.000498	0.053873	0
	Med.	8.795848	0.003875	0.054344	0
	High	1.187473	0	0.054244	0

Table 4-18: Sum of the Changes for All Cells in the Area Affected by Ground to Surface Water Transfers

Response Variable	Water Extraction Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [m]	Low	-0.0403	-0.3359	-0.3328	-0.3976
	Med.	-1.223	-2.9441	-4.0256	-3.6126
	High	-35.7362	-21.6811	-29.8735	-14.7325
SURFACE_WATER [m]	Low	-0.4173	0.0434	0.0047	-0.0151
	Med.	0.3944	0.9924	0.1382	1.214
	High	17.0222	11.0198	11.6827	4.4416
DIN_SF [g/m²]	Low	-1.2139	0.3715	-0.0468	0.0147
	Med.	-3.5364	1.583	0.5797	0.9814
	High	-11.8482	-3.6408	-0.4723	-2.4418
TOT_NPP [g/m²]	Low	1013.2	-64.8	-4.3	-4.0
	Med.	1697.3	-27.5	-36.9	-25.0
	High	3844.8	-170.9	19.0	39.7

Table 4-19: Number of Cells Affected by Ground to Surface Water Transfers for the Stated Intensities

Response Variable	Water Extraction Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [affected cells]	Low	131	130	132	121
	Med.	162	162	242	140
	High	237	232	239	192
SURFACE_WATER [affected cells]	Low	120	147	133	133
	Med.	139	161	152	146
	High	177	187	186	166
DIN_SF [affected cells]	Low	199	206	215	183
	Med.	230	236	287	199
	High	321	288	308	243
TOT_NPP [affected cells]	Low	45	49	39	20
	Med.	60	67	97	28
	High	108	102	127	56

Table 4-20: Average Magnitude of Change for a Response Variable in an Area Affected by a Ground to Surface Water Transfers

Variable	Intensity	Location 1	Location 2	Location 3	Location 4
SAT_WATER [m / affected cell]	Low	-0.0003	-0.0026	-0.0025	-0.0033
	Med.	-0.0075	-0.0182	-0.0166	-0.0258
	High	-0.1508	-0.0935	-0.125	-0.0767
SURFACE_WATER [m / affected cell]	Low	-0.0035	0.0003	0	-0.0001
	Med.	0.0028	0.0062	0.0009	0.0083
	High	0.0962	0.0589	0.0628	0.0268
DIN_SF [g/m2*affected cell]	Low	-0.0061	0.0018	-0.0002	0.0001
	Med.	-0.0154	0.0067	0.002	0.0049
	High	-0.0369	-0.0126	-0.0015	-0.01
TOT_NPP [g/m2*affected cell]	Low	22.5	-1.3	-0.11	-0.0217
	Med.	28.3	-0.4	-0.3802	-0.8919
	High	35.6	-1.7	0.1496	0.7093

4.5.4 Results: Different Disturbance Sizes and Shapes

Three patterns described in Section 4.1.5 are applied to the first location with a cumulative intensity equivalent to that of one high intensity disturbance. So, the high intensity water extraction with surface release value is divided among four cells for the square, line and distributed patterns. Response variable values are contained in Table 4-21 through Table 4-23. These tables present data meant to shed light upon the influence of industrial disturbance patterns on the modeled ecosystem.

Table 4-21: Sum of Magnitudes for Patterns of High Intensity Extraction and Release at Location 1

Pattern	Response Variables			
	SAT_WATER [m]	SURFACE_WATER [m]	DIN_SF [g/m2]	TOT_NPP [kg/m2]
Square	-117.3689	40.1908	-97.6334	4.6039
Line	-106.177	34.9217	-52.8429	3.8957
Distributed	-115.942	38.7081	-78.9975	4.0271

Table 4-22: Number of Cells Affected by High Intensity Extraction and Release at Location 1

Pattern	Response Variables			
	SAT_WATER [affected cells]	SURFACE_WATER [affected cell]	DIN_SF affected cell]	TOT_NPP [affected cell]
Square	252	188	333	119
Line	244	189	322	115
Distributed	257	193	336	118

Table 4-23: Average Change for Response Variables Affected by High Intensity Extraction and Release at Location 1

Pattern	Response Variables			
	SAT_WATER [m]	SURFACE_WATER [m / affected cell]	DIN_SF [g/m2*affected cell]	TOT_NPP [kg/m2*affected cell]
Square	-0.4657	0.2138	-0.2932	0.0387
Line	-0.4352	0.1848	-0.1641	0.0339
Distributed	-0.4511	0.2006	-0.2351	0.0341

4.5.5 Discussion of Results

Results obtained by observing the ecosystem model's response to groundwater extractions and accompanying surface releases are discussed. Changes in the four observed state variables serve as the focal point for the discussion. Where meaningful, comparisons between results in this experiment and results observed in the initial water extraction experiment explored in Section 4.3 are drawn.

Saturated water levels largely tend to drop in the vicinity of groundwater withdrawal points for every location, which supports the first hypothesis. For example, Table 4-18 shows that the first location experiences changes of -0.3976, -3.6126 and -14.7325 m for

low, medium and high intensity extractions, respectively. And, the top row of images in Figure 4-11 reveals that saturated water differences cluster around the point of extraction for the three intensities at all four locations. However, this trend does not apply to every cell. A few cells along surface water tracks experience saturated water increases as a result of infiltration. Comparing the final saturated water states for the groundwater extraction experiment with the experiment under discussion, one discovers that infiltration slightly increases the amount of water remaining in the extraction cells (See Table 4-6 and Table 4-17). Consider the final state of groundwater at the first location when subject to a high intensity extraction. When ground water is extracted but not released on the surface, 1.027508 m of saturated water remain in the extraction cell (See Table 4-6). When groundwater is extracted and released, 1.027628 m of water remain in the cell – an increase of 0.12 mm (See Table 4-17). The slight rise illustrates that surface water can infiltrate to the saturated zone during the time span of the simulation. It also reveals the at least qualitative similarity between the model and reality; pumped groundwater is not spilled upon earth during well tests because infiltration to unconfined aquifers can skew the results (Hudak 1999). *Surface water levels in the creek increase, and the extraction cells experience flooding. The presence of flooding lends credence to the second hypothesis.* At the highest extraction intensity, one does not observe flooding in the extraction cell during the 365th time step. Surface water values at the four extraction points listed in Table 4-17 all register zero values for high intensity extractions. The absence of flooding is a result of exhausting the groundwater supply in the extraction cell earlier in the simulation (See Table 4-7). Cells adjacent to the extraction cell often do not experience flooding. Interestingly, many of the scattered terrestrial changes in

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surface water amounts represent decreases. The low intensity runs for locations one and four actually result in net surface water losses (Table 4-18)!

Nitrogen pattern changes are rather complex. Many areas experience declines in surface nitrogen, but a few register increases. Location one experiences nitrogen changes of -1.2139, -3.5364 and -11.8482 g/m^2 for low, medium and high groundwater extraction intensities, respectively, but location two experiences 0.3715, 1583 and -3.6408 g/m^2 for the same intensities (See Table 4-14).   With the exception of location three, the geographic extents of nitrogen changes are similar to those observed for the groundwater extraction experiment (See Figure 4-11 and Figure 4-5).   Average surface nitrogen changes depend upon location and intensity (See Figure 4-12).
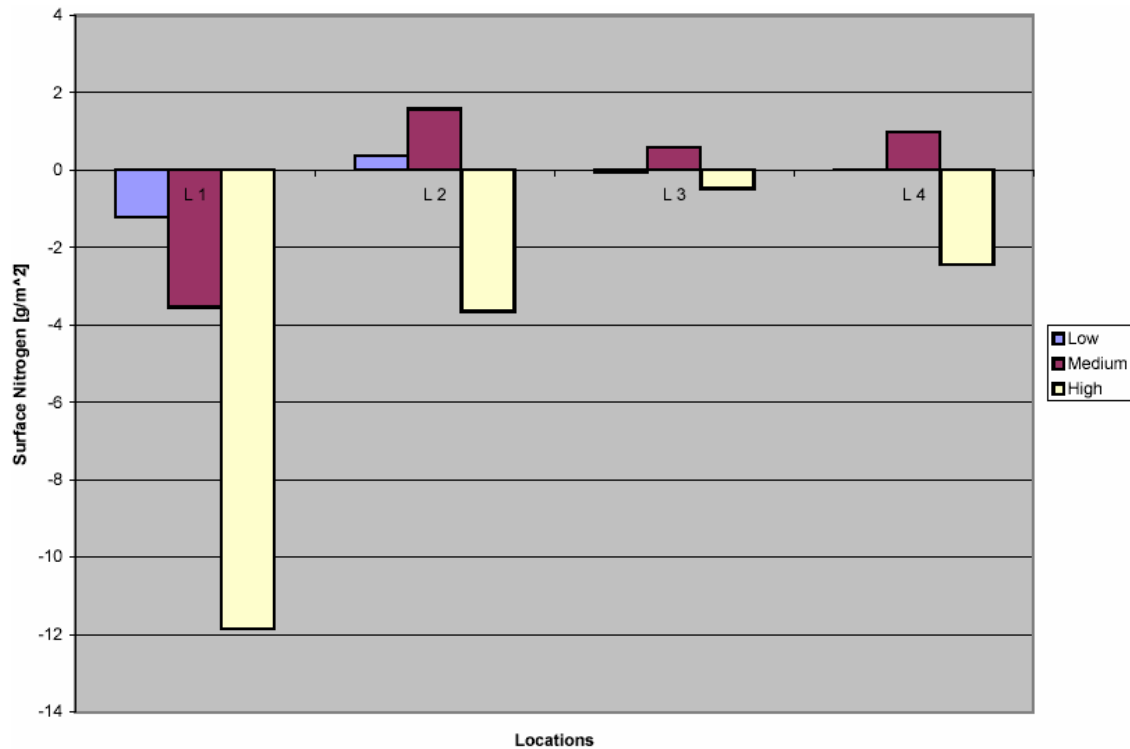
Figure 4-12: Surface Nitrogen for Three Intensities vs. Location

Location one experiences average nitrogen losses at all intensities while locations two and four only experience losses at the highest extraction and release intensities. Pattern

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disturbances experience nitrogen changes similar to those observed for a single disturbance at the first location (See Table 4-21 and Table 4-23). High intensity extractions cause average net losses regardless of location. Since the average losses exceed those for only groundwater extraction, high intensity surface releases appear to compound surface nitrogen losses from the watershed. Low and medium intensities tend to increase the amount of surface nitrogen in the system.

The geographic extent of changes reveals an interesting characteristic about the medium intensity water withdrawal and release for location three. For the saturated water and surface nitrogen variables, Figure 4-11 shows a wide blue swath of cells to the right and left of the central track taken by runoff. As a result, a disturbance at location three causes nitrogen changes in more cells for each of the intensities than any other location; at location three, low intensity causes changes in 215 cells, medium causes 287 and high causes 308. It is likely that cells to the right and left of the runoff track represent additional runoff tracks made possible by the combination of release and precipitation runoff. *The presence of changes in nitrogen patterns supports the third hypothesis.* These runoff paths are not utilized by the high intensity extraction because it exhausts the supply of groundwater in the extraction cell early in the simulation. This result tends to indicate that the frequency of an industrial disturbance is potentially as or more important than its magnitude.

Figure 4-11 reveals that NPP changes roughly center upon the point of extraction. *In the case of location three, the changes also correspond to the path taken by runoff en route to Hunting Creek. This finding supports the fourth hypothesis.* The values creating the patterns vary in magnitude; some cells suffer NPP drops while others gain.

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Comparing Table 4-10 and Table 4-20, one finds that groundwater losses dominate a majority of the NPP responses. NPP gains for the high intensity disturbance at location one for the first (35.7 g/m^2*affected cell) and third (35.6 g/m^2*affected cell) experiments differ by only 0.28%. While ground water changes cause the most significant effects, the persistent presence of surface water does cause the expected decline in NPP. The extraction cell, a point constantly submerged for medium intensity extractions, suffers a NPP decline. Some cells along the runoff track also experience NPP declines. *So, one finds evidence favoring the flood induced NPP decreases predicted by the fifth hypothesis.* The fact that not all cells in the runoff track suffer NPP losses is of note; it is a limitation of importance for the answer to thesis question 3d. The SME algorithm used to model the movement of runoff executes time steps smaller than one day (Voinov, et al. 1999b). If the macrophyte module updates at one day time steps, an underestimation of the impacts of flooding could result. Runoff would appear in only a handful of cells along a runoff track, and consequently, only those cells would experience the negative effects of flooding, despite the presence of water in the entire runoff course.

Results presented in Sections 4.5.3 and 4.5.4 generally support the hypotheses stated in Section 4.5.1. Multi-cell disturbances differ only in magnitude when compared to the corresponding single-cell disturbance. Ground and surface water respond in an expected manner, which supports an affirmative answer to question 3c. Infiltration mitigates the extent of flooding. And, the movement of surface water plays an important role in changing surface nitrogen patterns. Seemingly in contrast to the relevant hypothesis, changes in surface water have little impact on average NPP. The observed changes in NPP largely appear the consequence of groundwater reductions. Overall, this

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information adds to the growing body of evidence favoring a positive answer to question 3a. Trends present in the presented data add to the answer to question 3b.

4.6 Experiment 4: Gathering of Biomass for Industrial Use

Section 4.6 is the first of two sections devoted to industrial disturbances that directly affect biomass. In this section, a model for industrial biomass extraction is explored. The model assumes that industries gather biomass from a number of locations for the purposes of power generation and pulp and paper manufacturing. Ecosystem responses in terms of changes in non-photosynthetic biomass, surface nitrogen and NPP are observed. Then, these observations are compared with hypothesized ecosystem responses.

4.6.1 Hypotheses

When compared with the undisturbed Hunting Creek model, one would hypothesize four changes as a result of gathering biomass from the landscape.

1. First, the amount of non-photosynthetic biomass in the region of extraction should decline.

2. As a result of biomass losses, NPP should also decrease.

3. Increasing the intensity of biomass gathering should result in larger non-photosynthetic biomass and NPP drops.

4. One would also anticipate a rise in the amount of surface nitrogen in the system. Less plant growth translates into less demand for nitrogen; so, more nitrogen should remain in the system.

4.6.2 Biomass Gathering Intensity Justification

In the biomass gathering experiment, three different intensities of biomass extraction impact four different locations. The levels correspond to the daily amount of wood biomass required to supply power generation stations and pulp and paper manufacturers. At 500 ton/day, pulp and paper provides a high intensity figure, and at 75 ton/day, a power station's consumption provides the medium figure. Since medium intensity is roughly on-sixth of high intensity and a compelling low intensity use of biomass is lacking, low intensity is taken as one-sixth of medium intensity (12.5 tons/day).

4.6.3 Results: Single Biomass Gathering Point

Section 4.6.3 contains the results of extracting biomass at three different intensities from four different locations in the Hunting Creek watershed. Significant figures for response variable values appear in **bold** in the tables. The ecosystem response is summarized in the form of non-photosynthetic biomass (MAC_NPH_BIOMAS), surface nitrogen (DIN_SF) and total net primary productivity (TOT_NPP) changes. Table 4-25 holds the time required to effectively deforest a target cell given a specific extraction intensity.
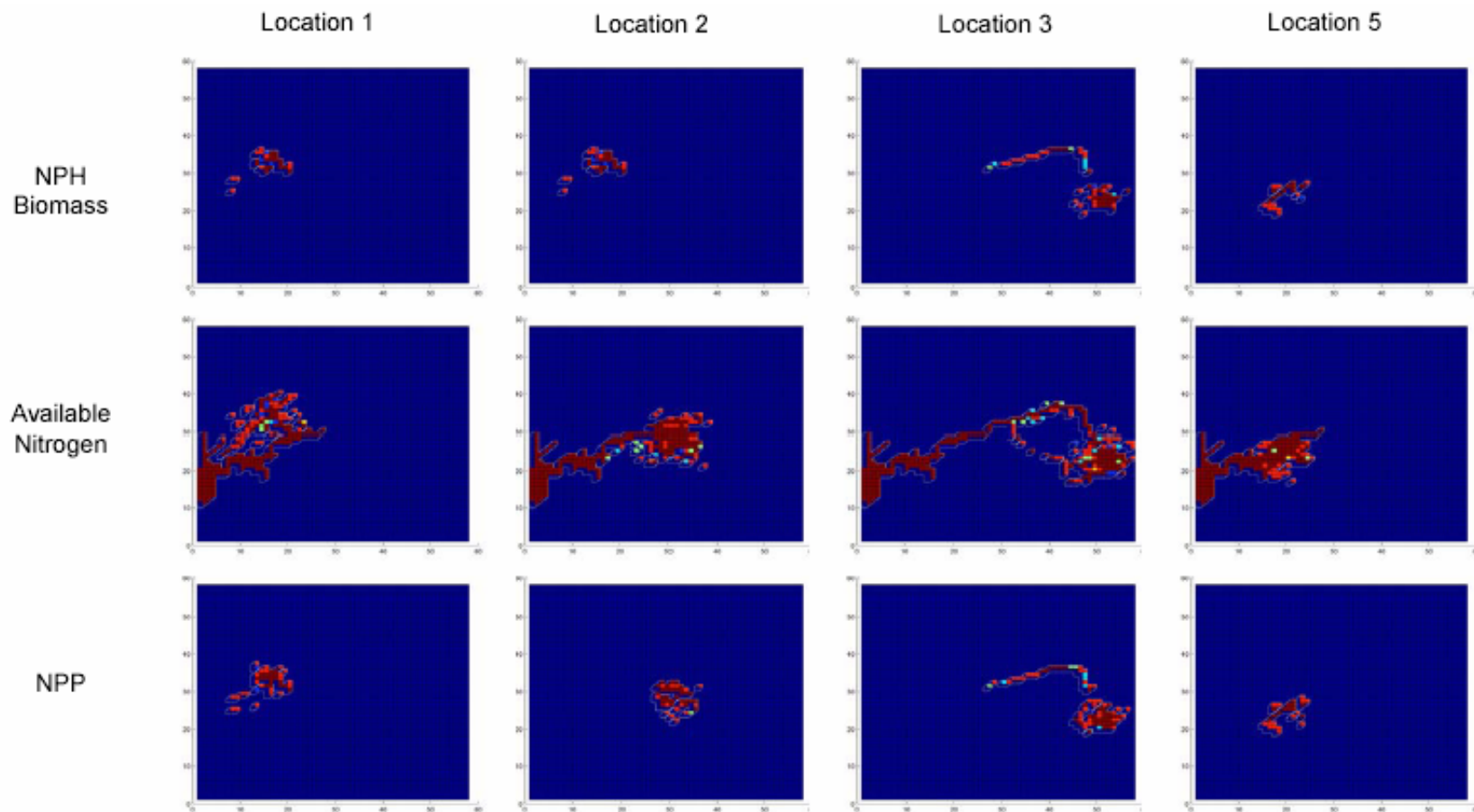
Figure 4-13: Geographic Extent and Pattern of Changes for NPH Biomass, Surface Nitrogen and (NPP) at Four Different Locations in the Hunting Creek Watershed When Subject to a Biomass Gathering Disturbance

Table 4-24: Final State of Cells Disturbed by Biomass Gathering

Location	Biomass Gathering Intensity	Non-Photosynthetic Biomass [kg/m²]	Surface Nitrogen [g/m²]	NPP [kg/m²]
#1 (25,15)	Low	**0.2**23908	**0.2**23122	**5.0**7861
	Med.	**0.1**22036	**0.2**23489	**0.0**10167
	High	**0.7**35349	**0.2**23434	**0.0**62148
#2 (30,30)	Low	**0.0**82804	**0.1**04624	**5.7**59338
	Med.	**0.2**82622	**0.0**9062	**0.1**73467
	High	**1.4**21855	**0.0**92162	**0.7**58593
#3 (35,50)	Low	**0.0**12061	**0.0**98167	**6.2**65321
	Med.	**0.4**11661	**0.2**38917	**0.3**05444
	High	**1.7**79086	**0.2**42	**1.1**24527
#5 (32,18)	Low	**0.0**97053	**0.1**58	**6.6**45304
	Med.	**0.4**00067	**0.1**09497	**0.2**94016
	High	**1.9**95556	**0.1**37328	**1.3**45831

Table 4-25: Time to Initial, Total Deforestation of a Cell (days)

Intensity	Location 1	Location 2	Location 3	Location 5
Low	174	175	176	174
Med.	27	27	27	27
High	4	4	4	4

Table 4-26: Sum of the Changes for All Cells in the Area Affected by Biomass Gathering

Response Variable	Biomass Gathering Intensity	Location 1	Location 2	Location 3	Location 5
MAC_NPH_BIOMAS [kg/m²]	Low	**-47.9**03	**-50.0**309	**-50.1**728	**-50.3**643
	Med.	**-48.1**225	**-49.8**087	**-49.5**612	**-49.8**634
	High	**-47.5**092	**-48.6**626	**-48.3**4	**-48.3**859
DIN_SF [g/m²]	Low	**-3.0**942	**-0.0**098	**0.0**377	**-0.0**607
	Med.	**0.8**994	**0.4**059	**0.3**761	**-0.0**161
	High	**0.8**833	**0.3**901	**0.3**573	**0.0**09
TOT_NPP [g/m²]	Low	2.5775	1.465	1.897	1.9924
	Med.	-2.614	-4.0987	-3.8462	-4.1572
	High	-2.5621	-3.5065	-3.1769	-3.2258

Table 4-27: Number of Cells Affected by Biomass Gathering for the Stated Intensities

Response Variable	Biomass Gathering Intensity	Location 1	Location 2	Location 3	Location 5
MAC_NPH_BIOMAS [affected cells]	Low	20	25	26	11
	Med.	27	36	56	21
	High	27	36	53	21
DIN_SF [affected cells]	Low	161	177	206	152
	Med.	197	212	254	175
	High	198	215	252	176
TOT_NPP [affected cells]	Low	20	29	33	12
	Med.	41	43	74	27
	High	41	44	72	27

Table 4-28: Average Change for a Response Variable in an Area Affected by a Biomass Gathering for the Stated Intensities

Response Variable	Biomass Gathering Intensity	Location 1	Location 2	Location 3	Location 5
MAC_NPH_BIOMAS [kg /m2*affected cell]	Low	-2.3951	-2.0012	-1.9297	-4.5786
	Med.	-1.7823	-1.3836	-0.885	-2.3744
	High	-1.7596	-1.3517	-0.9121	-2.3041
DIN_SF [g/m2*affected cell]	Low	-0.0192	-0.0001	0.0002	-0.3993
	Med.	0.0046	0.0019	0.0015	-0.0918
	High	0.0045	0.0018	0.0014	0.0513
TOT_NPP [g/m2*affected cell]	Low	0.1289	0.0505	0.0575	0.166
	Med.	-0.0638	-0.0953	-0.052	-0.154
	High	-0.0625	-0.0797	-0.0441	-0.1195

4.6.4 Results: Different Biomass Gathering Patterns and Extents

Three patterns described in Section 4.1.5 are applied to the first location with a cumulative intensity equivalent to that of one high intensity disturbance. So, the high biomass gathering value is divided among four cells for the three patterns. Response variable values are contained in Table 4-29 through Table 4-31. These data are meant to shed light upon the influence of biomass gathering patterns on the modeled ecosystem.

Table 4-29: Sum of Magnitudes for Patterns of High Intensity Gathering at Location 1

Pattern	Response Variables		
	SURFACE_WATER [m]	DIN_SF [g/m2]	TOT_NPP [kg/m2]
Square	-192.5644	3.017	-12.1103
Line	-191.7905	1.6329	-11.384
Distributed	-194.0912	2.4147	-13.6133

Table 4-30: Number of Cells Affected by High Intensity Gathering at Location 1

Pattern	Response Variables		
	NPH_BIOMAS [affected cells]	DIN_SF [affected cells]	TOT_NPP [affected cells]
Square	36	226	58
Line	37	224	55
Distributed	46	232	68

Table 4-31: Average Change for Response Variables Affected by High Intensity Gathering at Location 1

Pattern	Response Variables		
	NPH_BIOMAS [kg/m2 affected cell]	DIN_SF [g/m2*affected cell]	TOT_NPP [kg/m2*affected cell]
Square	-5.349	0.0133	-0.2088
Line	-5.1835	0.0073	-0.207
Distributed	-4.2194	0.0104	-0.2002

4.6.5 Discussion of Results

As one would expect, non-photosynthetic biomass decreases when compared with the undisturbed model. For example, the greatest differences between the undisturbed response and the responses resulting from gathering at locations 1-3 and 5 are -48.12, -50.03, -50.17 and -50.36 kg/m^2, respectively (See Table 4-26).
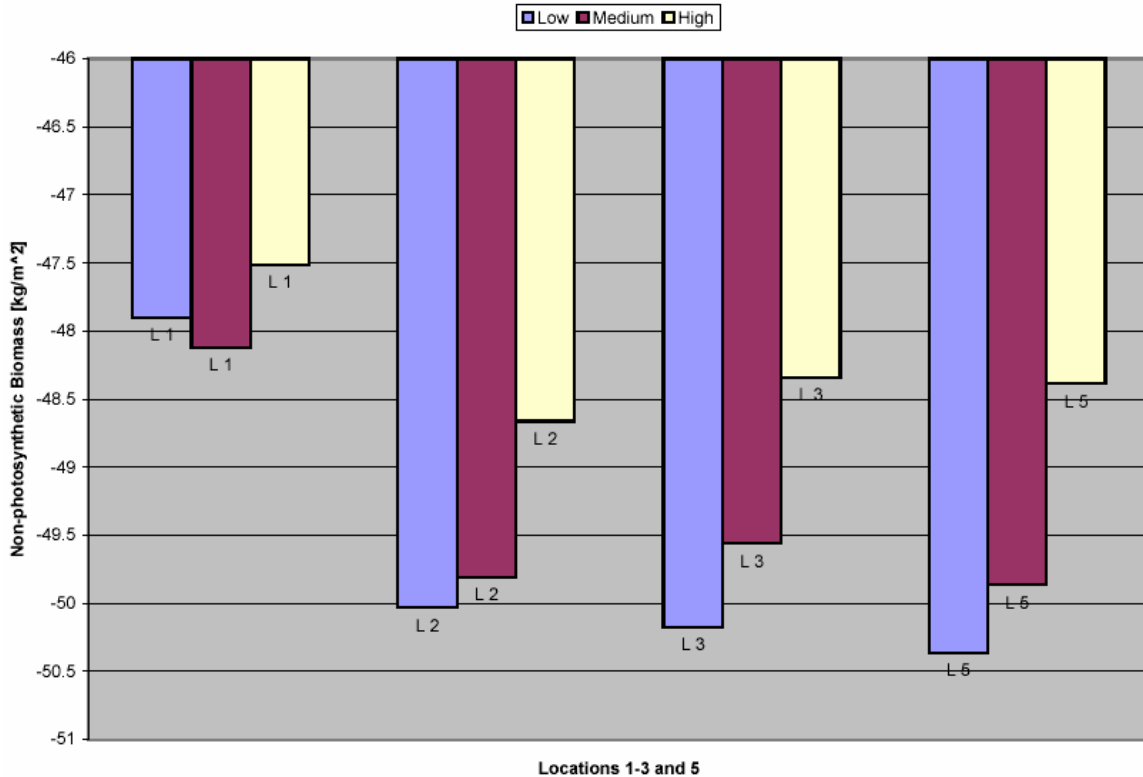
Figure 4-14: Non-photosynthetic Biomass Losses for Three Intensities vs. Location 1-3 and 5

The drop in non-photosynthetic biomass supports the first hypothesis. Interestingly, the size of the decline is not proportional to gathering intensity; in three of the four locations presented in Figure 4-14, the lowest intensity actually causes the highest loss. This discrepancy is largely the result of the discrete nature of the gathering events. Each gathering event occurs once per day if enough biomass is in the target cell. Gathering stops when non-photosynthetic biomass falls to a level smaller than the amount gathered in one event. Gathering resumes if biomass grows back to a level larger than the amount gathered in one event. Since the lowest intensity takes smaller increments, it can more completely gather biomass from a target cell, thus causing a larger drop. Table 4-28 illustrates the same behavior; at location five, the average biomass loss appears especially high. At the fifth location, low intensity gathering causes an average change of -4.58

kg/m^2*affected cell as opposed to average changes of approximately -2 kg/m^2*affected cell in the other locations. The high average results from the limited number of cells affected at the fifth location. Table 4-27 shows that low intensity gathering only changes non-photosynthetic biomass levels in 11 cells as opposed to more than twice that number for disturbances in the other locations. Geographic extent is limited by the fifth location's adjacency to Hunting Creek. Since creek cells lack standing biomass, they do not register changes in non-photosynthetic biomass. As with the water experiments, the high intensity multi-cell extraction patterns positioned near location one gather more biomass than the equivalent intensity in one cell because multiple cells sustain gathering longer than one cell (See Table 4-29 and Table 4-31). The data in Table 4-25 illustrate the predictable relationship between harvesting intensity and the length of time required to deforest a cell.

The response of non-photosynthetic biomass reveals the limitations of the representation for gathering; it adds to the answer to thesis question 3d. As mentioned, the behavior illustrated in Figure 4-14 is a result of incremental gathering. A more likely scenario involves the conversion of the entire 200 m^2 forested cell into a clear-cut cell during a single time step. Such a scenario depends upon the currently unavailable clear-cut land type. To better model the gathering of woody biomass, future representations should support discrete harvesting and replacement of forest cells with clear-cut cells.

Increases in surface nitrogen were expected for disturbed cells as a result of decreased uptake by plants. Suppressed uptake is a consequence of reduced plant growth. For medium and high intensity harvesting, the hypothesis holds; increases in surface nitrogen correspond with decreases in NPP (See Table 4-26, Table 4-28 and Table 4-29). Low

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intensity harvesting bucks the trend with net nitrogen losses in three of four locations. For locations one, two and five, increases in NPP and associated nitrogen uptake might explain the observed nitrogen reductions. However, the area influenced by gathering at the third location experiences a nitrogen gain of 0.0377 g/m^2 despite posting a NPP increase of 1.897 g/m^2 (See Table 4-26). Location five experiences a decrease in both surface nitrogen and NPP. The decrease in surface nitrogen despite biomass losses may result from increased erosion in cells deprived of ground cover. Loss of plant ground cover leads to a decrease in Manning Coefficient which in turn causes an increase in surface water flow rate (Fitz, et al. 1996). Interestingly, the square and distributed patterns exhibit significantly different nitrogen gains despite losing the roughly the same amount of biomass in roughly the same location. The system gains 2.41 g/m^2 of surface nitrogen when subject to the distributed disturbance and 3.02 g/m^2 when subject to the square disturbance (See Table 4-29). This result shows the influence of industrial patterns on ecosystem function.

For medium and high gathering intensities, NPP declined in comparison to the undisturbed model. NPP changes caused by gathering at location two are typical of changes at the other three. As Table 4-26 shows, low intensity gathering at location two caused a 1.47 g/m^2 rise while moderate and high gathering respectively caused -4.10 and -3.51 g/m^2 changes relative to the undisturbed model. Interestingly, medium gathering intensity demonstrated the greatest drops in all four locations (See Figure 4-15).
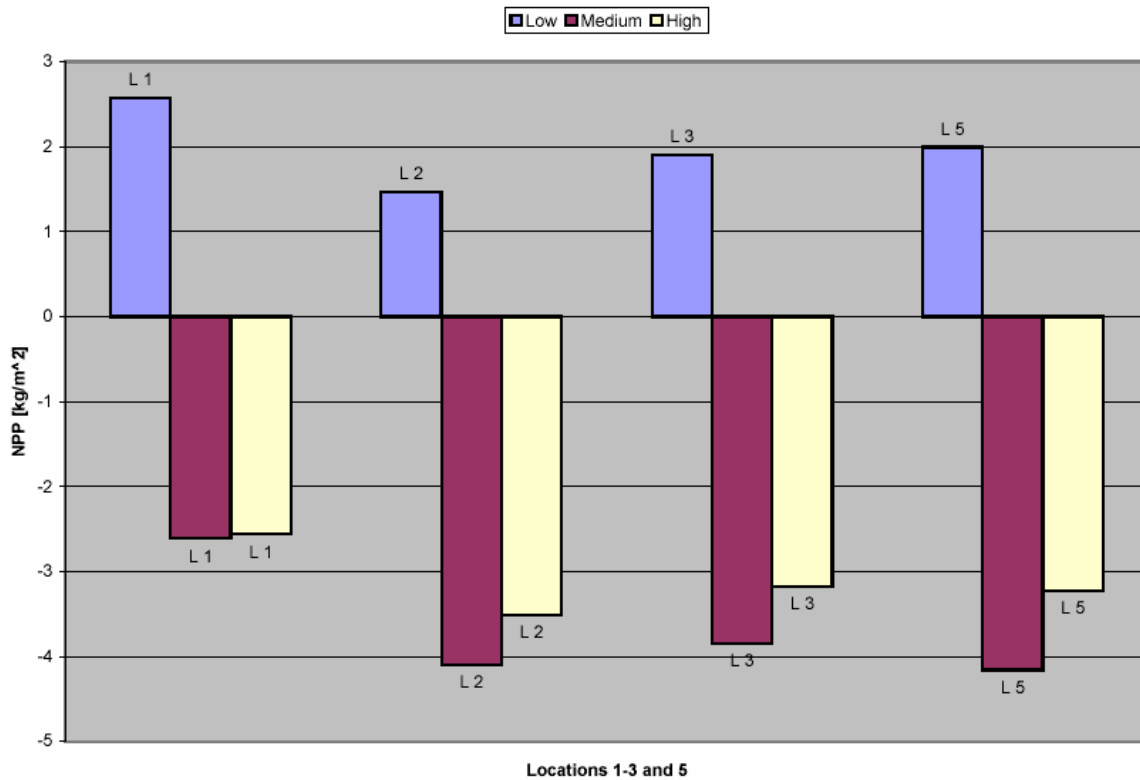
Figure 4-15: NPP for Three Intensities vs. Locations 1-3 and 5

This more severe decline is a consequence of the higher non-photosynthetic biomass losses and speed of depletion caused by medium intensity gathering. Note in Table 4-24 that medium intensity gathering causes the second highest non-photosynthetic biomass losses. Combining the low final level with the speed with which it reaches this level, one arrives at the reason behind the seemingly illogical result. High intensity reaches a minimum biomass level faster than medium intensity as shown in Table 4-25, but it leaves a larger standing stock of biomass. Low intensity more slowly approaches zero; so, the original stock has more time for photosynthesis. Medium intensity enjoys neither of these benefits; so, NPP achieves a minimum.

In defiance of expectations, NPP increased for the lowest gathering intensity. Despite significant non-photosynthetic biomass losses, plants actually grew more in the disturbed

cell than in the baseline cell! The form of the mathematical function that describes net primary productivity makes this paradoxical result possible. Net primary productivity, the derivative of net primary production, is defined as an inverse parabolic function of photosynthetic biomass with roots at zero and a defined maximum photosynthetic biomass (Voinov, et al. 2002). Figure 4-16 is a plot of the general form of the curve produced by such a function. One can see that net primary productivity rises to a maximum with the amount of photosynthetic biomass and then falls as it approaches the maximum allowable photosynthetic biomass.
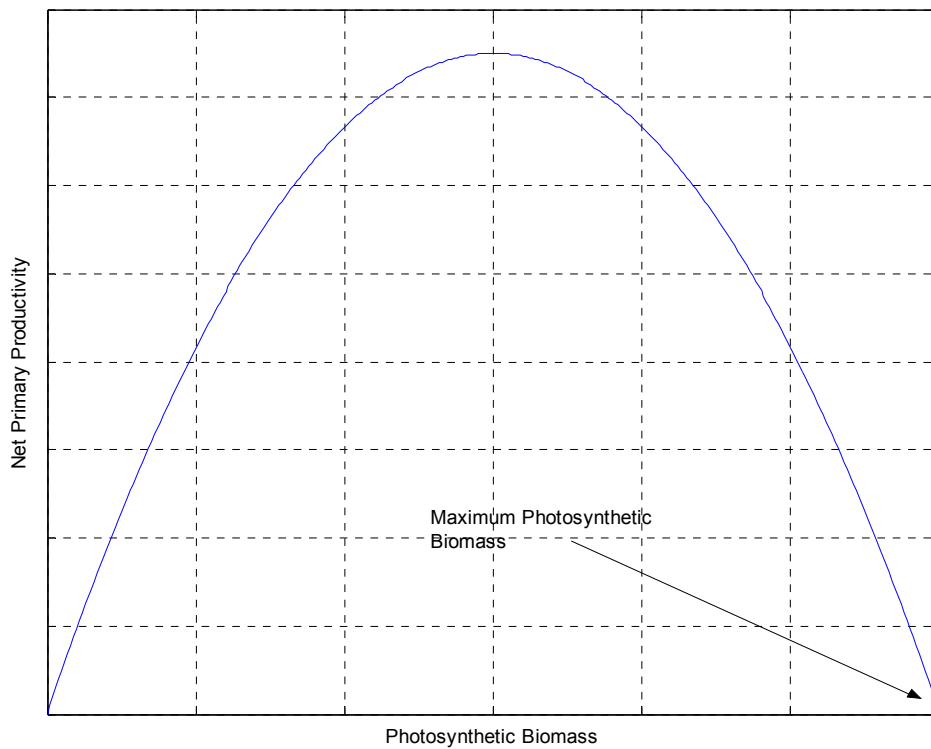
Figure 4-16: General Form of the Net Primary Productivity Function

As photosynthetic biomass approaches its maximum, the rate of net primary production decreases; so, reductions in this type of biomass would initially increase the rate of net

primary production. Reductions in non-photosynthetic biomass cause reductions in photosynthetic biomass which, when not severe, can cause increases in net primary production for the one year time period. Therefore, the rise in NPP at low intensity biomass gathering is quite plausible.

Upon comparing hypotheses with numerical results, one finds significant disagreement. While non-photosynthetic biomass decreases as hypothesized, surface nitrogen and NPP behave in an unanticipated manner. Furthermore, the ecosystem response to biomass gathering intensities reveals a trend at odds with expectations. In the case of NPP, one can explain the observed behavior by considering the size of the harvesting increment and the shape of the net primary productivity function. Explanations for surface nitrogen behavior, however, remain elusive.

The fact that biomass changes are detectable adds credibility to the running answer to question 3a. Trends, regardless of expectation, contribute to the answer to question 3b. The expected change in non-photosynthetic biomass and the reasonable explanation for NPP behavior contribute to answering question 3c in the affirmative.

4.7 Experiment 5: Industrially Induced Macrophyte Mortality Disturbances

The second of two sections dealing with direct, industrially induced biomass disturbances of the ecosystem, Section 4.7 investigates the result of introducing higher plant mortalities ostensibly caused by industrial pollution. An eco-toxicology model is not used; instead, the influence of pollution is simply represented as an increase in mortality for a given cell. Observations of the ecosystem response are compared with

anticipated system reactions in terms of non-photosynthetic biomass, deposited organic matter (DEP_ORG_MAT), surface nitrogen and NPP.

4.7.1 Hypotheses

In the fifth experiment, five hypotheses concerning the response of the system to elevated macrophyte mortality are investigated.

1. Non-photosynthetic biomass should decrease.

2. Consequently, NPP should also fall.

3. High mortality should raise the level of dead organic matter deposited in the affected cell.

4. Decomposition of dead organic matter releases nutrients; so, one should observe higher amounts of surface nitrogen.

5. Finally, each of these trends should prove more pronounced at increased levels of mortality.

4.7.2 Justifying Macrophyte Mortality Rates

Pollutant type and concentration play a role in determining changes in mortality (Jorgensen, et al. 1996).   Different mortality levels represent the influence of concentration, but since this experiment is a general investigation of the influence of mortality, a particular type of pollutant is not selected. Instead, the natural mortality level is scaled to generate the different pollution mortality levels. The low level mortality of $5.3x10^{-8}$ is one-tenth of the natural mortality. Ten times the natural mortality, $5.3x10^{-6}$, serves as the medium intensity, and the high level, $5.3x10^{-5}$, is set as 100-times natural mortality.

4.7.3 Results: Macrophyte Mortality as an Individual Disturbance

This section contains the results of simulating three different levels of industrially induced mortality in four different locations. The observed ecosystem response takes the form of changes in non-photosynthetic biomass (MAC_NPH_BIOMAS), deposited organic material (DEP_ORG_MAT), surface nitrogen (DIN_SF) and total net primary productivity (TOT_NPP). Significant figures for the response variables appear in **bold** in the tables.
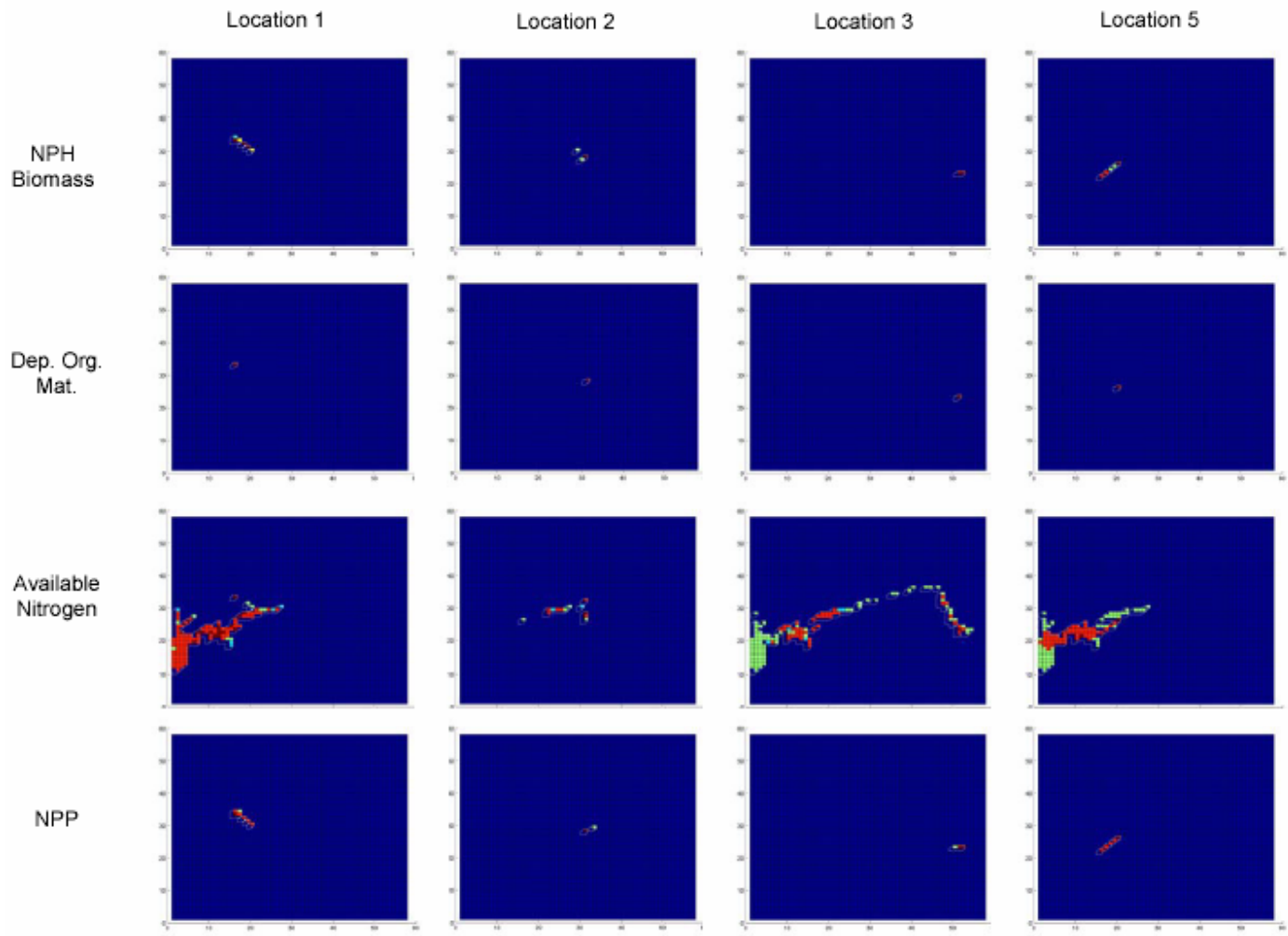
Figure 4-17: Geographic Extent and Pattern of Changes for NPH Biomass, Deposited Organic Matter, Surface Nitrogen and NPP at Four Different Locations in the Hunting Creek Watershed When Subject to Increased Mortality

Table 4-32: Final State of Cells Disturbed by Increased Mortality Levels

Location	Mortality Level	Non-Photosynthetic Biomass [kg/m^2]	Deposited Organic Material [kg/m^2]	Surface Nitrogen [g/m^2]	NPP [kg/m^2]
#1 (25,15)	Low	48.133739	0.952947	0.20093	2.508687
	Med.	48.132275	0.953039	0.201092	2.508846
	High	48.115795	0.953875	0.202568	2.510351
#2 (30,30)	Low	50.119488	0.953015	0.119005	4.300329
	Med.	50.118404	0.953107	0.119073	4.301064
	High	50.107357	0.953942	0.119733	4.307779
#3 (35,50)	Low	50.184669	0.953401	0.105183	4.367805
	Med.	50.183651	0.953493	0.105321	4.368499
	High	50.172195	0.954329	0.106223	4.374873
#4 (32,18)	Low	50.462914	0.953281	0.167899	4.654438
	Med.	50.461639	0.953372	0.167955	4.654902
	High	50.448177	0.954209	0.168463	4.659136

Table 4-33: Sum of the Changes for All Cells in the Area Affected by Industrially Induced Mortality

Response Variable	Mortality Level	Location 1	Location 2	Location 3	Location 4
MAC_NPH_BIOMAS [kg/m^2]	Low	0	0	0	0
	Med.	-0.0014	-0.0011	-0.001	-0.0013
	High	-0.0177	-0.0121	-0.0122	-0.0146
DEP_ORG_MAT [g/m^2]	Low	0.001	0.001	0.001	0.001
	Med.	0.093	0.093	0.093	0.092
	High	0.928	0.928	0.929	0.929
DIN_SF [g/m^2]	Low	0	0.000001	0	0
	Med.	0.002	0.00007	0.0002	0.0002
	High	0.021	0.000738	0.0014	0.0023
TOT_NPP [g/m^2]	Low	0	0	0	0
	Med.	0.0002	0.0007	0.0007	0.0005
	High	0.002	0.0075	0.0073	0.0048

Table 4-34: Number of Cells Affected by Industrially Induced Mortality at the Stated Levels

Response Variable	Mortality Level	Location 1	Location 2	Location 3	Location 5
MAC_NPH_BIOMAS [affected cells]	Low	1	1	1	1
	Med.	4	1	2	3
	High	5	3	2	5
DEP_ORG_MAT [affected cells]	Low	1	1	1	1
	Med.	1	1	1	1
	High	1	1	1	1
DIN_SF [affected cells]	Low	16	1	1	2
	Med.	107	9	48	56
	High	111	11	125	111
TOT_NPP [affected cells]	Low	1	1	2	1
	Med.	6	1	2	5
	High	7	2	3	5

Table 4-35: Average Change for a Response Variable in an Area Affected by the Stated Levels of Industrially Induced Mortality

Response Variable	Mortality Level	Location 1	Location 2	Location 3	Location 5
MAC_NPH_BIOMAS [kg /m2*affected cell]	Low	0	0	0	0
	Med.	-0.0004	-0.0011	-0.0005	-0.0004
	High	-0.0035	-0.004	-0.0061	-0.0029
DEP_ORG_MAT [g /m2*affected cell]	Low	0.001	0.001	0.001	0.001
	Med.	0.093	0.093	0.093	0.092
	High	0.929	0.928	0.929	0.929
DIN_SF [g/m2*affected cell]	Low	0.000001	0.000001	0.000002	0.000001
	Med.	0.0000188	0.00000778	0.000003670	0.00000423
	High	0.0001894	0.00006709	0.00001119	0.00002097
TOT_NPP [kg/m2*affected cell]	Low	0.000002	0	0	0.000003
	Med.	0.0000327	0.0007	0.0004	0.000096
	High	0.0002811	0.0037	0.0024	0.0009628

4.7.4 Results: Different Patterns and Extents of Macrophyte Mortality

Three patterns described in Section 4.1.5 are applied to the first location with a cumulative intensity equivalent to that of one high intensity disturbance. So, the high mortality value is divided among four cells for each of the patterns. Response variable values are contained in Table 4-36 through Table 4-38.

Table 4-36: Sum of Magnitudes for Patterns of High Mortality at Location 1

Pattern	Response Variables			
	NPH_BIOMAS [kg/m2]	DEP_ORG_MAT [g/m2]	DIN_SF [g/m2]	TOT_NPP [kg/m2]
Square	-0.0137	0.931	0.0115	0.0046
Line	-0.0138	0.93	0.0116	0.0044
Distributed	-0.0121	0.932	0.0068	0.0065

Table 4-37: Number of Cells Affected by High Mortality at Location 1

Pattern	Response Variables			
	NPH_BIOMAS [affected cells]	DEP_ORG_MAT [affected cells]	DIN_SF [affected cells]	TOT_NPP [affected cells]
Square	9	4	123	10
Line	6	4	115	9
Distributed	8	4	122	11

Table 4-38: Average Change for Response Variables Affected by High Mortality at Location 1

Pattern	Response Variables			
	NPH_BIOMAS [kg/m2*affected cell]	DEP_ORG_MAT [g/m2 *affected cell]	DIN_SF [g/m2*affected cell]	TOT_NPP [kg/m2*affected cell]
Square	-0.0015	0.2328	0.0000938	0.000456
Line	-0.0023	0.2325	0.0001007	0.0004918
Distributed	-0.0015	0.233	0.0000556	0.0005888

4.7.5 Discussion of Results

As expected, non-photosynthetic biomass stocks decrease, and the drops are greater for progressively higher mortality levels. Taking the first location as an example, differences with the baseline range from negligible at low mortality to -0.0177 kg/m^2 at high mortality. *This result yields evidence favoring the first and fifth hypotheses.* The changes are quite small and confined to the disturbed cell or a handful of cells in the vicinity of the disturbed cell; at most, even the highest mortality level only affects five cells (See Table 4-34). At the low mortality level, the model reports negligible biomass losses, and even at nearly 100 times the natural mortality, the highest loss is less than 20 g/m^2. Applying the same high mortality disturbance in the form of a multi-cell pattern

results in smaller non-photosynthetic biomass losses; the greatest change reported in Table 4-36 is -14.8 g/m^2. The discrepancy is likely explained by considering the fact that NPP is higher for the pattern disturbances than for the single disturbance.

Increased biomass losses cause increases in deposited organic matter, as stated in hypothesis three (See Table 4-33 and Figure 4-18).
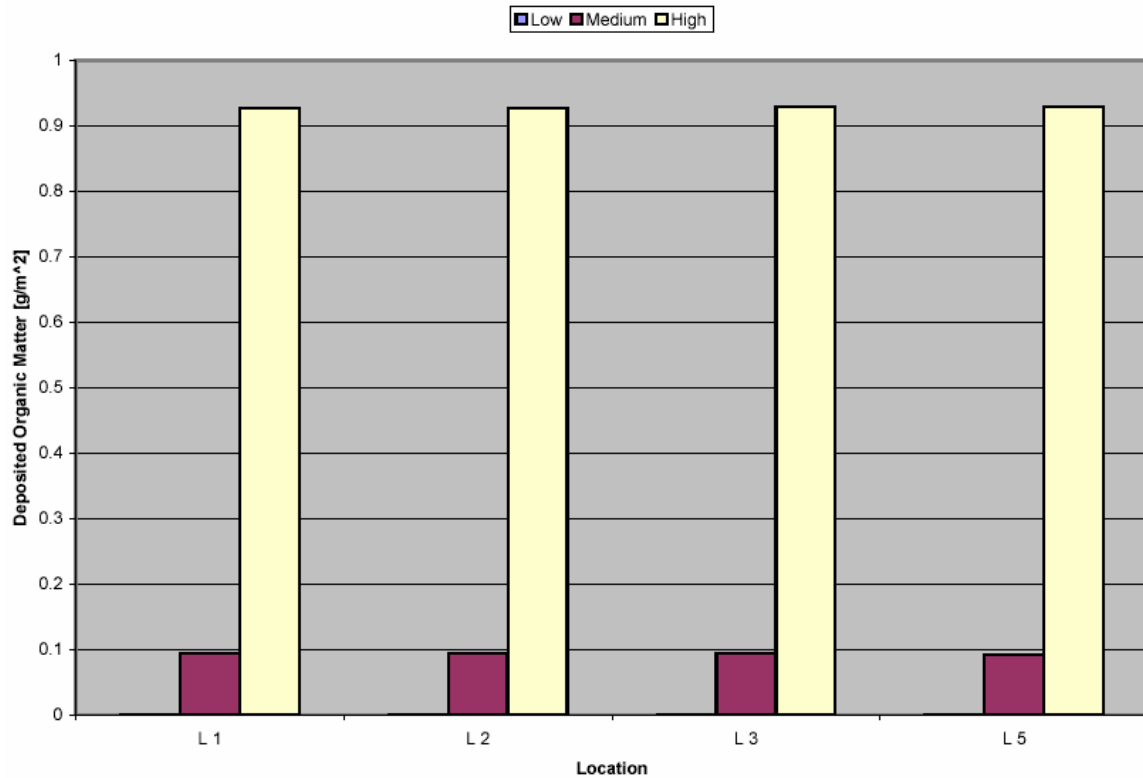
Figure 4-18: Deposited Organic Matter for Three Intensities vs. Location

However, the correspondence is not one to one. High mortality at location one reduces non-photosynthetic biomass by 17.7 g/m^2 when compared with the baseline, but deposited organic material increases by only 0.928 g/m^2 (See Table 4-33). Though one might expect the mass lost by forested cells to appear as deposited organic material, this is not the case.   The modeled decomposition process first allows dead matter to degenerate into labile and stable detritus, and then, some of the stable detritus becomes

deposited organic material (Voinov, et al. 2002). As a result, only a fraction of lost non-photosynthetic biomass actually becomes deposited organic material. Different biomass losses result in nearly the same amounts of organic material; even disturbance patterns possess nearly equivalent values (See Table 4-36). The similarity in values results from the fact that mortality is modeled as a fraction of the standing non-photosynthetic biomass and that the stock values only vary by a few percent during the simulation.

The rise in surface nitrogen is an anticipated system response. The model allows for the return of nutrients to the system by decomposition (Voinov, et al. 2002). So, the increase in available dead organic matter leads to a rise in nitrogen. The size of the rise varies with intensity, location and disturbance pattern. When one compares the amount of nitrogen in the system for a high intensity, single cell disturbance at location one with the pattern disturbances, one discovers that the pattern disturbance nitrogen values are lower by as much as a factor of three. Though small, Table 4-34 reveals that the change in nitrogen affects a significant geographic area for three of the four disturbed locations; Table 4-37 shows that this observation also holds for the patterns. Many of the cells experiencing nitrogen changes are part of Hunting Creek. The widespread differences with the baseline model result from the fact that runoff can move surface nitrogen into the creek. *Taken together, these observations provide confidence in the correctness of the fourth hypothesis.*

Despite non-photosynthetic biomass losses, the disturbed model experiences slightly higher amounts of plant growth in all four locations for most of the intensities. These positive changes are another instance of increasing net primary productivity by decreasing photosynthetic biomass as explained in Section 4.6.5. If one included the

influence of toxins on germination and growth, one might see different results; one would expect decreased NPP resulting from increased mortality coupled with suppressed germination and growth. Pattern disturbances register NPP gains exceeding that of the corresponding single cell disturbance. Higher NPP is a likely explanation for the smaller net non-photosynthetic biomass losses and smaller amounts of surface nitrogen.

The results of the experiment support four of the five hypotheses stated in Section 4.7.1. Non-photosynthetic biomass levels fall, and the amount of deposited dead organic matter rises. Surface nitrogen levels increase. And, the response magnitude proves proportional to the mortality level for all four variables. However, the results run counter to the hypothesis concerning NPP; NPP increases with increasing non-photosynthetic mortality levels. The NPP increases likely result from productivity increases associated with small biomass declines, as previously mentioned. For all of the response variables, multi-cell disturbance patterns cause trends similar to single-cell disturbances.

However, one must consider the mortality link both a technical success and a practical failure. Though results corroborate many of the hypotheses, a vast majority of the supporting evidence takes the form of data beneath the significant figure threshold set in Section 4.2.2. Ecosystem model inaccuracies and ecosystem data uncertainties fatally limit the mortality link.

4.8 Verification of Results

Support for the reasonableness of the results presented in Chapter 4 comes in three forms. The fact that the work depends upon a previously verified ecosystem model and the conservation of mass principle provides the primary support. Qualitative

comparisons to literature and expected physical responses serve as a second support form. And, review of the document by a systems ecologist lends the third form of support. In Sections 4.8.1-4.8.3, these three forms of support are discussed in greater detail.

4.8.1 Verified Models

The validity of the results presented in the previous sections depends upon the reasonableness of the models which produced them. These models consist of an ecosystem landscape model with mass flow modifications meant to represent the inputs and outputs of industrial facilities. So, results verification depends upon establishing the truth and reality of the ecosystem landscape model and the conservation of mass principle.

Mass conservation is an accepted principle with overwhelming empirical support. The modifications to the ecosystem model presented in Section 3.3 are soundly rooted in principle of mass conservation; consequently, they are valid in a physical sense. As discussed in Section 2.3.4, researchers and practitioners successfully use mass conservation to produce representations of industrial facilities that prove useful when identifying environmental burdens. So, these modifications are appropriate in terms of decision support as well.

Representing ecosystems with ecosystem landscape models is a far less certain endeavor than representing industrial flows using a form of the conservation of mass principle. Consequently, any ecosystem representation requires significant verification before one can accept model outputs. The Patuxent Landscape Model and associated Hunting Creek watershed model are not exceptions to this requirement. The creators of these models embarked upon an extensive verification effort involving the major model components as well as the assembled model.

Costanza and coauthors first verified the unit model and spatial hydrology, and then, they verified the entire model (Costanza, et al. 2002). The creators verified the unit model for a landscape type by comparing model outputs with 1) ecosystem data stored in independently generated databases, 2) known qualitative trends and 3) the output of previously verified models. In the case of comparison with other models, they report coefficient of determination (R^2) values between 0.87 and 0.98 (Costanza, et al. 2002). They used data and an existing model to compare and verify the spatial hydrology for the PLM. They compared stream flow data gathered from United States Geological Survey gaging stations with PLM spatial hydrology outputs, and they compared outputs from the Hydrologic Simulation Program-Fortran (HSPF) model with results produced by the PLM. Having compared the PLM with data and other model outputs, Costanza and coauthors found that the "…general hydrologic trends seem to be well captured by the model…" (Costanza, et al. 2002). Having verified the unit model and the spatial hydrology model, they next verified the assembled model by comparing its outputs to time series and spatial data. They found good agreement the assembled model and the available data (Costanza, et al. 2002).

Use of an accepted principle, mass conservation, and a well verified ecosystem landscape model, the PLM, contributes significantly to the validity of results presented in Sections 4.3-4.7 and claims made in Section 4.9.

4.8.2 Literature and Physical Reasoning

Literature and physical reasoning serve as another form of verification. In this section, the role of literature and physical reasoning in verifying the results in Sections 4.3-4.7 is described. By understanding the use of literature and physical reasoning, the

reader gains a measure of confidence in the results not afforded by basing the validity of the work solely upon the validity of its component parts.

Each experiment contains a section devoted to a set of hypotheses that the experiment tests. By testing these hypotheses, one primarily gains evidence that aids in answering the third thesis question. Hypotheses with especially obvious answers also aid in results verification. For example, consider the first hypothesis in Section 4.3.1. If one draws water from the ground, physical reasoning dictates that a decline in water level near the point of extraction will result. Model responses showing something besides a local decline would be viewed with suspicion. Since physical reasoning reveals the qualitative form of the system response, one possesses a sound basis for comparing the results of testing these simple hypotheses with the eco-industrial model. One achieves a rough level of qualitative verification by comparing the obvious, expected system response with the modeled response. Correspondence between the two helps verify the model.

Qualitative trends noted in the literature also facilitate eco-industrial model verification. Comparing model outputs to observed, qualitative ecosystem trends noted in the literature allows one to check the correspondence between representation and reality. For example, consider the plot of saturated water near the point of groundwater extraction shown in Figure 4-9. The surface corresponds to plots of saturated water levels in the vicinity of wells noted in the literature (Hudak 1999). When outputs match trends noted in the literature, one gains confidence in the model.

4.8.3 A Systems Ecologist's Perspective

The final form of verification is a review of the thesis by Dr. Alexey Voinov. As one may have gathered from the citations, Dr. Voinov is a chief modeler for the PLM. His

experience with PLM creation, calibration and verification allows him to look upon the modeling component of this work with the keen eyes of an expert. His comments about the work do not suggest that the results in Chapter 4 are invalid.

However, he did raise an important cautionary point. Without empirical data corresponding to the situations investigated in the experiments, one cannot be certain that the model results are correct. The best way to achieve this level of certainty is to build an industrial system that causes the defined disturbances in Hunting Creek watershed. One could then gather data and compare it with modeled outputs. Unfortunately, this course of action is prohibitively expensive and time consuming. One must settle for the somewhat ambiguous verification offered by basing eco-industrial modeling on verified models, qualitative verification of data trends and review by a master modeler.

4.9 Reviewing the Chapter and Connecting the Third Thesis Question

In this closing section of Chapter 4, experiments and results are cast within the context of the objectives for the chapter. The work is first related to the objective of testing eco-industrial model linkages, and then it is connected to the third thesis question.

4.9.1 Affirming Accomplishment of the Chapter Objective

In the fourth chapter, the functionality of the linkages proposed in the third chapter was evaluated using five experiments. In each of the five experiments, the industrial disturbances produce primarily comprehensible, though not necessarily intuitive, ecosystem responses. The results demonstrate the functionality of the location control, groundwater flow, surface water flow and biomass flow links proposed in Chapter 3 (See

Table 4-39).   Due to ecosystem model and data inaccuracies, one must consider the mortality link a technical success but a practical failure.

Table 4-39: Summarizing Functionality Tests

Link	Tested in Section(s)	Summary of Test Result
Location Control	4.3-4.7	The specified location is observed to experience the appropriate change.
Groundwater Flow	4.3 and 4.5	Saturated water levels fall when groundwater is extracted.
Surface Water Flow	4.4	Surface water levels fall when surface water is extracted.
Biomass Flow	4.6	Non-photosynthetic biomass levels decline as a result of gathering.
Mortality Fraction	4.7	Biomass losses increase with increasing mortality; however, a majority of the supporting data is insignificant.

Where results prove contrary to expectations, explanations based on physical reasoning or ecological modeling literature support the reasonableness of the results and illustrate the potential pitfalls of linear, intuitive thinking. The reasonableness of the results in turn builds confidence in the functionality of the elemental building blocks for eco-industrial models.

4.9.2 Connecting the Third Thesis Question

In addition to demonstrating functionality, the fourth chapter also contains the answer to the third thesis question, 'Can one currently detect the impact of industrial changes on the modeled ecosystems?' Sub-questions concerning the detection of impacts resulting from reasonable disturbances, patterns and trends and the correlation between results and reality are also addressed. For a few experiments, identification of model limitations also proves relevant.

The ecosystem response variable changes reveal that this type of ecosystem landscape model can indeed detect industrial disturbances. The verification discussion in Section 4.8 provides reasons to trust the listed results and related conclusions.

- Results in Sections 4.3.3 and 4.3.4 reveal that the model responds to changes in groundwater extraction rates.

- Data from Section 4.4.3 indicate that one may detect changes resulting from surface water extractions.

- Sections 4.5.3 and 4.5.4 contain data showing the detectable differences in the system caused by varying the rates at which groundwater is released on the surface.

- Sections 4.6.3 and 4.6.4 hold results indicating changes caused by the removal of biomass.

Since the magnitudes of these disturbances take values found in common industrial situations, the model can detect the impact of reasonable industrial situations as well.

- As discussed in Sections 4.3.2 and 4.6.2, the values used for ground and surface water extractions as well as biomass gathering are drawn from industrial sources. Therefore, the models can detect changes caused by input and output magnitudes found in industry.

- Three intensities of input and output disturbances are applied to the system. These intensities span one or more orders of magnitude in the value of the disturbance variable, and the ecosystem model registers a response at all intensity levels. However, not all observed model responses are significant. Given the wide disturbance range over which the model responds, one can

expect the model to detect the impact of management decisions that change disturbance levels by a few percent for industries responsible for high or medium disturbance flows. However, the model may not detect changes in industries classified as having low intensity flows.

The observed impact trends are discussed in the sections dealing with the individual experiments, and in most cases, these trends correspond to expectations or possess reasonable explanations.

- In Section 4.3.5, for example, the reader learns that the expected saturated water declines occur as result of groundwater extractions.

- Section 4.6.5 contains an explanation of the surprising rise in NPP caused by low intensity biomass harvesting. The section describes how the net primary productivity function interacts with biomass levels to produce this result.

Potential model limitations appear in the groundwater extraction, groundwater to surface water and mortality experiments.

- In the groundwater extraction experiment, the decline in saturated water magnitudes in cells surrounding the extraction point may not be realistic (See Section 4.3.5).

- The current runoff algorithm may limit the ability of the model to estimate the impacts of persistent industrial runoff as discussed near the end of Section 4.5.5.

- Changes registered by increasing mortality likely fall below the level that one can reliably predict with the current ecosystem landscape model.

In the fourth chapter, one learns the answer to the third thesis question and associated sub-questions. The brief review of the chapter in this section gathers and summarizes the elements of the answer revealed by the five experiments. Having answered the three thesis questions, the way is clear to summarize the thesis results and contributions in Chapter 5.

CHAPTER 5

Revisiting Questions, Clarifying Contributions and Charting a Future Course

The fifth and final chapter contains answers to thesis questions, a list of contributions a lessons learned and an introduction of possible, future research directions. In Section 5.1, each thesis question is restated and revisited. Section 5.2 contains a description of the work's primary contributions. Section 5.3 lists lessons. And, Section 5.4 outlines potential research paths.

5.1 Summarizing Answers to the Thesis Questions

The objective of research is to raise and answer questions. The purpose of this thesis is to answer three research questions. Table 5-1 contains these three primary questions and associated secondary questions that the three previous chapters attempt to answer. In the following sub-sections, the answers to these research questions are summarized, and lessons learned while answering these questions are discussed.

Table 5-1: Restatement of Primary and Secondary Thesis Questions

Primary Question	Secondary Questions
1. What characteristics should linked industrial and ecosystem models possess?	a. What are the uses and resultant defining characteristics of current environmental and ecological models?
	b. What are the uses and resultant defining characteristics of industrial facility models?
	c. What level of interaction does the environment have with industrial facilities?
2. How can one link ecological and industrial models?	a. What inputs and outputs link the two types of models?
	b. How can one represent these links using available tools?
3. Can one currently detect the impact of industrial changes on the modeled ecosystems?	a. Can one detect the impact of reasonable, industrial management decisions on the modeled ecosystem?
	b. If so, what response patterns and trends appear, if any?
	c. Do the predictions correlate with observed results or reasonable expectations?
	d. Are model limitations encountered?

5.1.1 Eco-Industrial Model Characteristics

Defining characteristics serves as the first step in the process of learning to build eco-industrial models. Section 2.2 describes the characteristics of six broad classes of environmental models, and Section 2.3 performs the same function for industrial models. To answer questions 1a and 1b, one must identify general model classes, motivations for building these models and model characteristics. The literature survey directly revealed environmental model classes as made evident in Table 2-1. A classification structure for industrial models was created in Section **2.3.1**. Each environmental and industrial model class is discussed in Sections 2.2.1-2.2.6 and **2.3.2-2.3.4**, respectively. These sections elucidate the reasons for and purposes of each model class. Because Sections **2.2** and

2.3 classify model types, identify motivations for building each model class and describe model characteristics, these sections answer Questions 1a and 1b. The discussion of mass flow models in Section **2.3.4** is of special interest because it reveals one of the classic ways industrial systems interact with the environment. The section shows the importance of mass flows that cross the boundary between industrial systems and the environment for representing interactions between the two systems. It is the foundation for the answer to Question 1c.

To answer the first primary thesis question, one must assemble and filter the characteristics for environmental and industrial models identified in Sections 2.2 and 2.3; one must filter the answers to 1a and 1b through 1c. Assembly and filtration occurs in Sections **2.4.1** and **2.4.2**. Requirements list headings selected with an eye to the answer to 1c filter the environmental and industrial model characteristics that populate the individual requirements lists. In Section **2.4**, the insights gained in the three prior sections combine in the form of general requirements lists for ecological and industrial systems models. The superposition of these two requirements lists is advanced as a set of characteristics for eco-industrial models. Because these lists contain the distillation of answers 1a-1c, Table 2-7 does indeed provide the answer to the first primary research question.

5.1.2 Linking Industrial and Ecological Models

Chapter 3 represents a practical approach to answering the second primary thesis question listed in Table 5-1. Instead of focusing upon the creation of multiple customized eco-industrial models, the chapter forges rudimentary links that one can reuse to embody multiple eco-industrial models. As a first step toward creating these reusable

links, Question 2a is answered. One answers this question by first identifying the environmental and industrial models worth linking and by then identifying the specific connections between the two models. Eco-industrial modeling requirements from Chapter 2 are mapped to existing ecosystem and industrial models in Section 3.1. The mapping process uses the requirements list to identify the models worth linking. Having identified and justified the selection of an ecosystem and an industrial model, the specific types of links implied by the mapping are made explicit in Section 3.2. Section 3.1 identifies models, and Section 3.2 specifies links. Together, these sections answer Question 2a. Question 2b is answered by describing the details involved with forging the links explicitly stated in Section 3.2. Section 3.3 describes implementing these links using STELLA software and the SME. The section shows the step-by-step processes used to create the links tabulated at the end of Section 3.2. Therefore, Section 3.2 answers Question 2b. The reader leaves chapter three with an understanding of how to link industrial and ecological models; the reader departs with the answer to the second primary thesis question.

5.1.3 Detecting Impacts

The experiments conducted on the Hunting Creek ecosystem landscape model in Chapter 4 reveal that the links proposed in Chapter 3 are functional and that one can indeed detect environmental impacts with these models. Results in Section 4.3 through 4.7 clearly show changes in ecosystem state variables as a result of the introduced industrial disturbances – answering the third primary thesis question. These sections also yield sufficient information to answer Questions 3a-d.

To affirmatively answer Question 3a, state variable changes must cause significant ecosystem responses at fractional disturbance magnitudes. This criterion is necessary because reasonable management decisions usually increase or decrease material outputs and / or inputs by a fraction of baseline usage. Data presented in Sections 4.3 to 4.6 reveals ecosystem responses ranging from low to high intensity. Facilities with high and moderate intensity consumption and emission could conceivably experience fractional changes ranging from low to moderate. Low to moderate changes cause significant model responses. The fact that the responses were elicited for disturbances on a scale of those actually found in industrial situations permits an affirmative answer to Question 3a. An answer to Question 3b requires trend identification. Trends appear for many of the response variables observed in Sections 4.3-4.6. In Sections 4.3 and 4.5, groundwater always drops in the vicinity of an extraction for example, and the severity of the decline varies proportionally with intensity extraction. NPP increases for low intensity harvesting regardless of location in Section 4.6. These and other trends serve as an answer to Question 3b.

One finds the answer to Question 3c by comparing model outputs with responses found in the literature and with those dictated by physical reasoning. As explained in Section 4.8, the most basic hypotheses in each experiment partially exist to test model outputs against physical reasoning. A number of response variables respond as one would expect; groundwater near extraction points drops for example. Literature is also used to check some response variable behavior. For example, one discovers that the shape of the groundwater curve first observed in Section 4.3 corresponds with that found in the literature. For response variables such as groundwater, surface water, non-

photosynthetic biomass and NPP, the model responds in predictable or, at least, explainable ways, but for surface nitrogen, this is not the case. The fact that model responses are corroborated by physical reasoning and literature permits a positive response to Question 3c.

In response to Question 3d, a potential limitation of the subsurface hydrology module is noted in Section 4.3. The nature of the surface run-off algorithm limits the usefulness of the model for predicting the impact of surface releases as mentioned in Section 4.5, and in Section 4.7, one discovers that model inaccuracies severely limit the mortality fraction linkage's usefulness.

However, one must remember that the experiments reported in Chapter 4 apply to one subwatershed for one weather pattern. One would need to conduct these experiments for multiple watersheds and weather patterns before one could attribute statistical significance to the current affirmative answer to the third research question. So, overall, Chapter 4 tentatively demonstrates that the proposed links produce detectable, believable ecosystem responses.

5.2 Listing and Describing Contributions

The previous thesis chapters make three contributions.

1. Identification, implementation and evaluation of rudimentary links between industrial and ecological system models compose the first contribution.

2. Establishment of the infrastructure needed to conduct dynamic, spatially explicit ecosystem modeling within the Environmentally Conscious Design and Manufacturing (ECDM) Program is the second contribution.

3. The final contribution is the creation of a collection of MATLAB programs needed to convert and manipulate ecosystem model outputs in a Microsoft Windows environment.

These three contributions are described in more detail in Section 5.2.1, 5.2.2 and 5.2.3.

5.2.1 Identification, Implementation and Evaluation of Model Links

Answers to the three thesis questions constitute the primary contribution of this work. These answers define the desirable characteristics of integrated industrial and ecological systems models, describe a means of linking the two types of models and test the functionality of these links. Each of these accomplishments makes a unique contribution to the general body of knowledge.

A set of necessary and desirable integrated model characteristics function as a goal. Within the context of the thesis, these characteristics guide development of the links between the two types of models. Since these characteristics are based upon a review of environmental and industrial modeling literature, they also serve as a justifiable end state toward which future efforts can develop eco-industrial models.

The links described in Chapter 3 contribute knowledge of how to connect industrial and ecological models. The premise of connecting these two types of models is not unique; in fact, many environmental models implicitly assume industrial disturbances in the form of mass flows. However, implementation of this premise using components of ecosystem landscape models and selected flows that one may readily connect to a particular facility is unique.

The final general contribution takes the form of an evaluation of the model links. By testing the linking methods for reasonable industrial disturbances, confidence in the

appropriateness of the method is built. The ranges of detectable impacts are clarified, and some of the potential weaknesses of the approach are exposed. In essence, the results in Chapter 4 contribute an understanding of how and when to use the set of building blocks, the links, created in Chapter 3.

Characteristics, links and evaluations are the general and most visible contributions of this thesis. However, they are not the only contributions. These achievements stand upon two other foundational achievements discussed in Sections 5.2.2 and 5.2.3.

5.2.2 Establishment of Spatial Modeling Environment Infrastructure

To create an eco-industrial model, one needs representations of both industries and ecologies. Training and education in engineering provided knowledge of industrial models, but the typical mechanical engineering education is devoid of experiences needed to create ecosystem models. So, this thesis relies upon ecosystem landscape models developed by the Gund Institute for Ecological Economics at the University of Vermont. Replicating the computational infrastructure needed to run and manipulate these models at Georgia Tech is the first local contribution of this thesis.

Though barely a mention of the effort to establish the Spatial Modeling Environment infrastructure appears in the body of the thesis, it is, nonetheless, foundational. One could not create or evaluate eco-industrial modeling links without a functional SME. Furthermore, future work in eco-industrial modeling would be curtailed without continued maintenance of this capability at Georgia Tech.

Appendices A and B contain a distillation of the knowledge gained while establishing the SME at Georgia Tech. Here, one finds information concerning both the installation and operation of the SME. The material contained in these appendices is in addition to

the installation and reference materials provided by the Gund Institute for Ecological Economics; therefore, it represents an independent contribution.

5.2.3 Post-Processing SME Data in Windows

Another local contribution takes the form of MATLAB code used to port, manipulate and analyze the raw data output by the SME. Appendix C contains a number of programs and sub-programs used to translate SME map outputs into mathematical arrays and to visualize translated data. Many of the sub-programs are MATLAB modules that one may readily reuse to support future analyses. The fact that the programs provide a way of porting the data from a Unix / Linux environment to a Windows environment is of special importance. With a means of porting the data available, one can spend less time developing computational infrastructure and more time conceiving experiments and analyzing data. Though not initially intended as a contribution, the aggregation of MATLAB code needed to solve various emergent problems has resulted in something of value in and of itself.

5.3 Lessons Learned

While striving to answer the thesis questions listed in Table 5-1, a number of observations not directly related to answering the thesis questions were noted. This section airs the most important of these lessons.

5.3.1 Environmental Blinders

As a consequence of the environmental impact focus of the work, the eco-industrial links appear directional. They appear to focus on the impact of industry on the environment while ignoring the impact of the environment on industry. The existence of

links such as biomass mortality certainly reinforces this observation. Links to groundwater, surface water and biomass possess a strong bi-directional character, however. The results in Sections **4.3**-**4.6** reveal the environmental impacts, and one can imagine the industrial impact of losing access to process water or raw materials in the form of biomass. Nonetheless, even these links possess an environmental bias. Beyond amounts, the biomass and water links do not provide additional industrially relevant information. For example, different biomass types have different heating values which effect industrial users in need of process heat.

5.3.2 Industrial Habitats

By creating eco-industrial links and working through the associated experiments, it was learned that available habitat types do not appropriately represent some industrial activities. During presentation of the biomass experiment in Section **4.6**, the need to create "industrialized habitats" became obvious. Forested cells reduced to nearly zero biomass remain forested cells in the current ecosystem model. Growth and other characteristics remained those of forests, even though the land has been emptied of trees. A superior representation would account for habitat changes caused by industrial activities. A forested cell could become a clear-cut cell during biomass extraction for example. A clear-cut habitat is one of a number of conceivable industrialized habitats that an eco-industrial modeler would wish to have available. Another habitat type is the industrial park. Industrial facilities can exceed 200 m^2; so, an industrial unit cell is needed to account for such facilities.

5.3.3 Model Inaccuracies

Another unexpected result of this study is an understanding of the limitations placed upon the predictive capacity of the model by inaccuracies. Though the model often responded to industrial disturbances, many responses to low level disturbances fall below the threshold set for significance in Section 4.2.2. Indeed, all results for the mortality link presented in Section 4.7 fall below the significance threshold. Such outcomes inform eco-industrial modelers that the utilized ecosystem model lacks the ability to predict ecosystem responses to small scale industrial operations. These results also argue in favor of developing alternate means of representing the impacts of toxic materials in the utilized ecosystem landscape model; adjusting mortality proves insufficient for predictive purposes.

5.3.4 Documentation – A Gap in Need of a Bridge

Current documentation for the SME does not span the full spectrum of user needs. When attempting to understand, install and use the SME and its supporting software, one currently finds two types of supporting documentation. Academic literature such as conference articles and journal papers aid one in understanding the output of models developed using the SME. Reference manuals and readme files, the second documentation form, provide minimal installation support and a list of commands. Unfortunately, the span between minimal installation support and fascinating model outputs remains in the minds of the modelers. Troubleshooting, model assembly and data structure explanation are three topics that must be addressed to bridge the existing gap.

Documenting troubleshooting requires documentation of potential installation problems and model assembly problems. Ideally, such documentation would indicate the meaning of error messages and suggest means of remedying the associated errors. An

explanation of the "debug level" feature is also needed; instruction in its prudent use is desired.

The model assembly procedure is not entirely clear in the current documentation. A step-by-step description of how to assemble an ecosystem landscape model when given its various pieces is needed. A tutorial is also needed. Given sample model components, the tutorial would demonstrate the use of the step-by-step procedure to assemble an ecosystem landscape model with the SME.

Finally, additional documentation should contain an explanation of the data structures used in SME models. Data structure documentation would include a description of the file structure for SME models as well as a description of the files themselves. File explanation would entail verbal and visual description so the structure of configuration files, time series data files, spatial data files and equations files.

5.4 A Future for Eco-Industrial Modeling

Potential, future, eco-industrial modeling work divides into three general categories: modeling, design and infrastructure improvements. Modeling work partitions into the creation of new modules and the improvement of the links between existing models. Design research would focus on applying existing models within the context of integrated product, process and landscape design. And, infrastructure improvements would center on achieving "modeling parity" with Vermont.

5.4.1 More Models

From the outset, the type of material flows modeled in the Hunting Creek and related ecosystem landscape models was recognized as a limitation. Industry passes metals, organic chemicals, ozone precursors and more to the environment in the form of effluents and emissions. However, the available ecosystem landscape models only account for naturally occurring materials such as water, nitrogen, carbon and phosphate. A new module dealing with the fate and transport of materials unique to industry would enhance the scope and usefulness of the current ecosystem landscape model framework. Though potentially fraught with difficulties, the development of an air shed to sit atop the currently modeled watersheds would allow modeling of the impacts of airborne emissions on local environments. These research objectives fall within the purview of eco-toxicologists, environmental engineers and systems ecologists, however.

Improvement of modeling links is work more accessible to engineers. One can make some link improvements by simply upgrading the modeling infrastructure as discussed in Section 5.4.3, but others require more fundamental research. The set of building block links proposed in Chapter 3 is not exhaustive; the ecosystem landscape model contains a number of additional variables one might manipulate to better represent the interface between the two systems. By coupling a number of existing industrial models to the ecosystem model using the developed building blocks, one might eventually see an opportunity for adding to the current set.

Extending the model to include the product system also represents a modeling research opportunity. As Figure 5-1a illustrates, the current eco-industrial model only links production facilities with local environments. One could foresee linking the

product system with a particular system that manufactures the product in a particular locale, as shown by Figure 5-1b. Or, one could attempt to model the use phase of a products life cycle by using life cycle inventory analysis data to connect the product system with the ecosystem model (See Figure 5-1c).
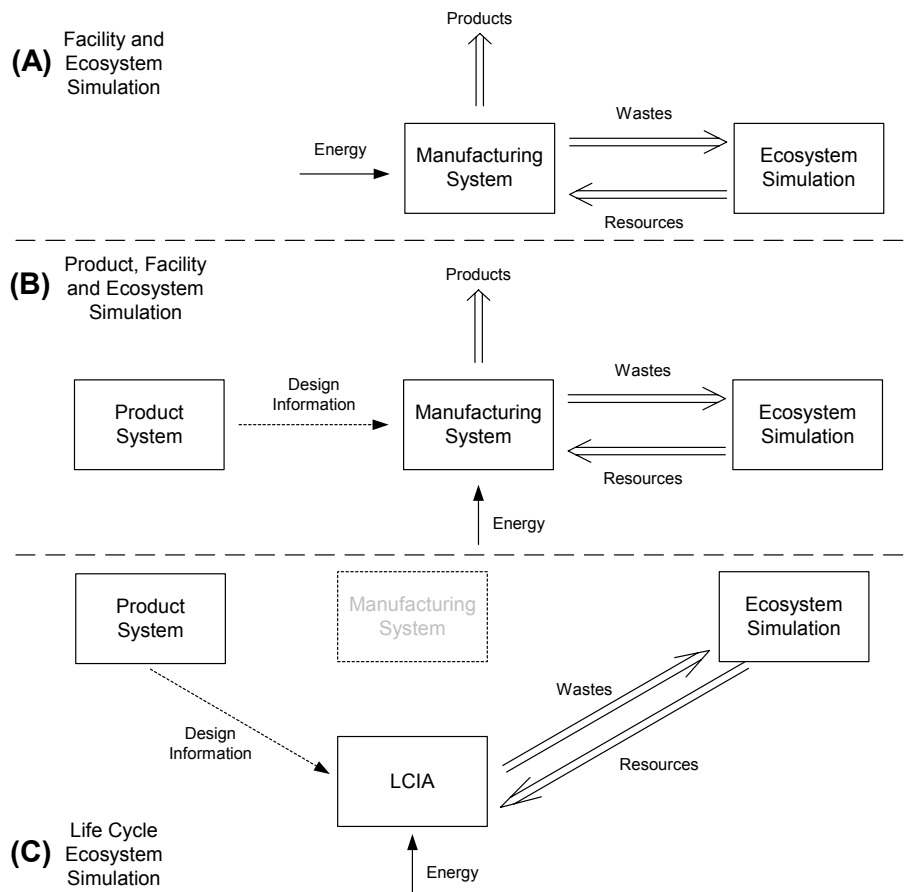
Figure 5-1: Opportunities for Eco-Industrial Model Extensions

Using spatially explicit, dynamic ecosystem landscape models in this life cycle capacity could potentially improve impact assessment problems related to the lumped sum parameter and steady state assumptions currently in use (Reap, et al. 2003).

5.4.2 Designing in the Space of Products, Processes and Landscapes

Research in eco-industrial system modeling is closely coupled with research in eco-industrial system design. The models create the space one explores in design. Research in design would focus on incorporating ecosystem landscape models into facility and product design. The overarching question is how to formally represent the simultaneous design of products, manufacturing processes and ecosystem landscape (See Figure 5-2).
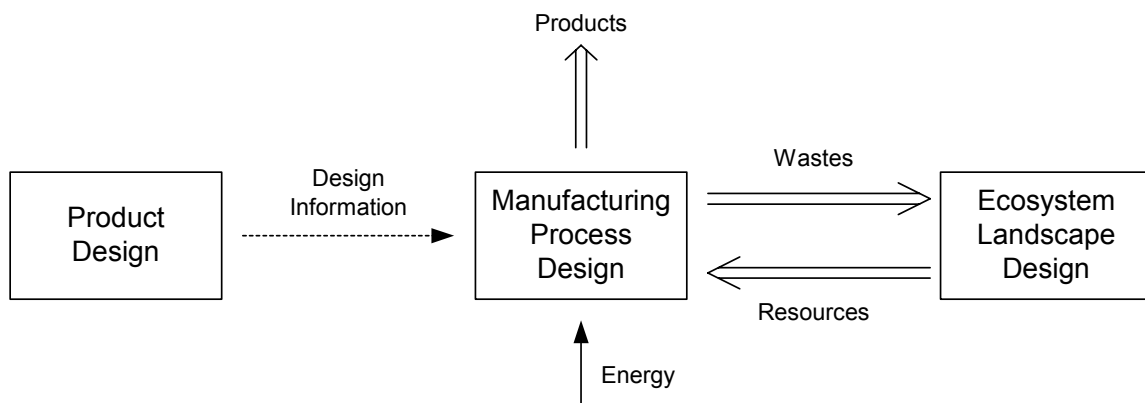
Figure 5-2: Connections Between Product, Process and Landscape Pattern Design

5.4.3 Of Dreadnaughts and Ecosystem Landscape Models

The final future work element involves equalizing the ecosystem modeling disparity between Georgia Tech and Vermont. While the current ecosystem modeling infrastructure at Georgia Tech provides the essential modeling functions, the activation of existing functions is both possible and necessary for continued work in eco-industrial modeling. For example, the current Hunting Creek habitat map cannot be edited because of the map format (Macintosh) and user code in the model. Exploration of the ecosystem landscape pattern design problem and the coupled product, process, pattern design problem require control of the habitat map. The habitat map problem and others like it could be remedied by a combination of acquisition and instruction. The acquisition of

hardware and software compatible with that used by the Gund Institute would alleviate format conflicts, and instruction about the inner workings of the SME would facilitate its application to modeling and design problems. However, it is important to realize that hardware and an increased knowledge base in no way replace input from Gund Institute members.

5.5 Closing Remark

Having developed the eco-industrial modeling project to the state revealed by the previous chapters and sections, I find, upon reflection, a certain kinship with the famous Spanish explorer Hernando de Soto. De Soto journeyed from Spain to the area of the southeastern United States lured by tails of riches waiting in the interior. I began my journey lured by riches as well; I set out in search of a wealth of new information. He explored territory in what would become Florida, Georgia, South Carolina, Alabama, Mississippi and Arkansas. I too wandered in strange and unknown territories, the territories of ecosystem science and linux platforms. The men in De Soto's expedition encountered, surveyed, noted, fought and suffered across miles of trackless wilderness, but they never found the riches they sought. The motivational goal of knowing if a region or locale is sustainable remains remote despite having surveyed literature, fought to forge links and suffered with research code. Yet, perhaps De Soto and I missed something.

Riches lure many. For me, the accounts of environmental impacts simulated in space and time were the lure. The papers spoke of complete, functional, tested models capable of reporting changes in nitrogen levels to the milligram. In ecosystem landscape modeling, I saw an opportunity to escape the vagaries of LCA and risk assessment.

Environmental impacts could be simulated; the uncertainties that led to confusion concerning the selection of paper or plastic bags at the market could be bypassed. I had but to traverse a little intellectual distance between Chapter 1 and Chapter 5.

A little distance became something more in time. The road to grasping the rudiments of ecosystem models, linux and the SME research code was traveled, and it did not prove smooth. Available references did not prepare me for what was to come. Efforts from software installation to model assembly proved rocky.

When at last the eco-industrial model links yielded results, uncertainty remained. The level of accuracy in outputs limited the predictive capacity of eco-industrial models based upon the utilized ecosystem landscape models. And, of course, doubt concerning the validity of the approach could not be completely erased unless one could compare the observed impact of an industry in the modeled region with the modeled impact of said industry. It would seem, then, that riches proved beyond the grasp of both De Soto and me.

The moral of the thesis resides in this point. The work of the previous four chapters is preliminary. It is a first exploration of an uncharted area – blue sky. The recommended paths may not be correct, but others need to spend time on the "land" to find the "coal," use the "pines" and benefit from its "fertility." It is my hope that this thesis, limited though it may be, takes the first of hopefully many steps in the eco-industrial modeling journey.

Appendix A

Creating Portable Pixel Maps (PPM) for Location Control

Appendix A provides information needed to create map variables that control the location of inputs from and outputs to the ecosystems in which industrial facilities are embedded. It is referenced in Section 3.3.1. Section A.1 details the format for portable pixel maps used to control facility locations in the Hunting Creek model. Section A.2 describes the simple process of editing these maps to change the location of inputs and outputs. Together, the two sections provide the reader with sufficient information to create and edit location control maps.

A.1 PPM Format for Facility Location Control in Hunting Creek

The beginning of a PPM file takes the following inset form. The first four lines control file type, size and accepted values. The remaining lines contain data.

```
P3
# this file controls location
57 57
1
0 0 0  0 0 0  0 0 0 …
0 0 0  0 0 0  0 0 0 …
  .        .        .
  .        .        .
  .        .        .
```

The first line defines the file type. Of the two types of PPM files, raw (P6) and plain (P3), the SME recognizes the rarer P3 format. The second line provides room for documentation; the number symbol comments the line. The third line defines the size of

the data array input on lines five and higher. In the Hunting Creek case, the entered array size is 57 by 57. A 57 by 57 array is actually a 58 by 58 array because the PPM file appears to start line and column counts at zero. Line four contains an integer indicating the maximum color value; the maximum color value is simply the largest integer value with which one can replace a zero in any of the data columns.

Lines greater than or equal to five contain location data. Each line contains elements of each column composed of three zeros. The position for the third zero in each element holds location data in the form of an integer. The elements in the PPM array correspond to cells in the Hunting Creek or other SME study area.

A.2 Examples: Modifying Maps to Control Facility Location

By changing the third zero in an element of a column, one controls the location of an input or output specified in one of the non-spatial modules from which one constructs an eco-industrial model. The value for the element in the PPM array is the value taken by a corresponding cell in a spatial variable configured using the PPM file. For example, changing the element in the second row and second column of a spatial variable to a value of one would require the following array.

```
P3
# this file controls location
57 57
1
0 0 0  0 0 0  0 0 0  …
0 0 0  0 0 1  0 0 0  …
.       .       .
.       .       .
.       .       .
```

Changing the value in the third column of the first row would require a slightly different PPM map.

P3
this file controls location
57 57
1
0 0 0 0 0 0 0 0 1 …
0 0 0 0 0 0 0 0 0 …
.   .   .
.   .   .
.   .   .

Appendix B:

Guidance and Procedures for Installing and Using the SME with a Red Hat

Linux 7.1 Operating System

Appendix B exists to assist novice Linux users in the installation of the SME and configuration of the Hunting Creek Landscape Model. Section B.1 provides installation guidance, and Section B.2 provides a detailed procedure for configuring a version of the Hunting Creek model ported from another UNIX-based operating system.

B.1 Guidance for Installing the SME

The intent of this section is to offer guidance to researchers with little knowledge of Linux / UNIX operating systems. It contains an overview of and tips and clarifications for the Spatial Modeling Environment installation procedure written by Maxwell in the distribution readme file (Maxwell 1995). It does not contain an independent procedure guaranteed to successfully install the SME within a different operating system.

B.1.1 Overview of the Procedure

Given that one is using a machine with all of the necessary supporting software, the installation procedure divides into four general steps:

Unpacking – The SME program (a.k.a. distribution) file is transformed from a compressed form to an uncompressed one.

Path establishment – The directory structures for the SME and potentially Java are made available at the command prompt.

Configuration – An installation script called a shell is used to configure the unpacked SME distribution.

Building – The configured distribution is built.

B.1.2 Important Procedural Details

Though seemingly simple, installation can become problematic for individuals uninitiated in the ways of Linux / UNIX. So, Table B-1 contains more detailed information about the procedure outlined in the previous section. Though the commands and comments therein are "old hat" for experienced Linux users, it is the hope of this author that they may prevent at least one novice from "seeing red" during the installation process.

Table B-1: SME Installation Tips

General Step	Specific Action	Example of Corresponding Command
Unpacking	Create a directory for the SME installation.	mkdir /usr/share/sme
	Copy the distribution to this directory.	cp /mnt/zip/sme-3.1.71 /usr/share/sme
	Unpack the distribution untar / unzip commands.	tar –xvzf sme-3.1.71
Path Establishment	Include the path for the SME binary files in the path for the user. (Note the syntax of the example command. The ":$PATH" component appends the existing path with the new directory structure. Without this closing command, the user path would be replaced by the input directory structure.)	export PATH=/usr/share/sme/bin:$PATH
	Include the path for Java	export PATH=/usr/java/j2sdk1.4.1_02/bin:$PATH

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	binary files in the path of the user.	
Configuration	Copy the install shell to the SME directory.	cp /mnt/zip/sme_linux_install.sh /usr/share/sme
	Edit the shell as specified in its documentation.	
	Execute the shell.	./sme_linux_install.sh
Building	Follow the directions written by Maxwell (Maxwell 1995).	make install
	One may need to create a few directories for the SME or to change the permissions on one or more directories.	

B.2 Procedures for Building and Configuring the Hunting Creek Model

This section focuses upon the configuration and building of a model based upon a model configured and built for a different UNIX platform. The purpose of the section is

- To explicitly document the procedure used to configure and build the Hunting Creek sub-watershed model

- To highlight and describe problems encountered during the configuration and building processes

- To reveal solutions and possible solutions to these problems

First, the assumptions underlying the content of this section are presented. Then, two procedures are introduced. The first procedure is a general approach for configuring and building models in the Spatial Modeling Environment (SME). The second procedure describes the steps taken, problems encountered and solutions applied to successfully configure and build the Hunting Creek model.

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B.2.1 Caveats and Assumptions

While reading Section B.2, one must remain mindful of the fact that the specific procedure, encountered problems and suggested solutions apply only to the Hunting Creek model run with SME 3.2.71 installed on a computer using Linux 7.1 as an operating system. These and other assumptions are documented in Table B-2. Despite these limiting assumptions, the general procedure for configuring and building remains valid, and the specific procedures and solutions should prove helpful to those engaged in preparing a different model or in preparing the same model for a different machine.

Table B-2: Basic Assumptions

#	Assumption	Comment
1.	Operating System: Linux 7.1	Reports of success running the SME on Linux 9.0 exist
2.	sme-3.2.71	The distribution as of 5/23/03 is sme-3.2.72
3.	SME configured using the "sme_linux_install.sh"	This is quite an effective method of configuring the SME, though it is rather difficult for the novice to successfully modify.
4.	Successful Installation of the SME	"Successful" often requires some qualification.
5.	Starting with the "Hunt.tar" file and separate "Model" and "UserCode" directories	The Hunt.tar file contains broken symbolic links to the Model and UserCode directories. Therefore, separate Model and UserCode directories are required.

B.2.2 General Procedure

To the best of this author's knowledge, one may apply the procedure presented in Table B-3 when configuring and building any model using the SME.

Table B-3: General Procedure for Configuring and Building a SME Model

Step	Description	Comment
1.	Create a SME project using the command, "SME project <proj. name goes here>"	

2.	Declare an SME model name using, "SME model <model name goes here>"	
3.	Copy data into the project's "Data" directory.	
4.	Copy equation files into the project's "Models" directory.	These files bare the extension ".eqns"; they are "*.eqns" files.
5.	Copy user defined C-code into the project's "UserCode" directory.	These files come in pairs. For example, C-code for surface water flow is accompanied by a header file. So, one would need to copy two files: "SWater.cc" and "SWater.h".
6.	Import the "*.eqns" files using the command, "SME import 1.eqns 2.eqns etcetera.eqns" for the first time.	
7.	Add user function links to the <model name goes here>.MML.Config file.	
8.	Import the "*.eqns" files using the command, "SME import 1.eqns 2.eqns etcetera.eqns" for the second time.	
9.	Name the scenario using the command "SME scen <scenario name goes here>".	
10.	Build the model using the command "SME build".	
11.	Link appropriate variables in the "<model name goes here>.conf" file	Do not forget the "~ Framelink" variable.

B.2.3 Specific Procedure

In Table B-4, the steps taken to configure and build the Hunting Creek model on the assumed system are listed and described. Confronted problems are noted, and solutions are detailed. Many of these problems were identified by observing command line outputs. Running the SME from the command line interface is preferred when initially debugging a model because the java interface produces ambiguous error messages.

Table B-4: Procedure for Configuring and Building the Hunting Creek Model

Step	Procedure	Problems and Solutions
1.	Copy "Hunt.tar" to /usr/share/sme2/Projects/. Note	

	$SME\_Home=/usr/share/sme2/$.	
2.	Untar "Hunt.tar" using "tar –xvzf Hunt.tar"	
3.	Copy the appropriate …/Models and …/UserCode directories to $SME_Home/Projects/HUNT	The symbolic links in the untarred HUNT directory are broken. The described manual copying procedure overcomes this minor problem.
4.	Go to $SME_Home/bin. Open the file "SME". Find the line "OPTFLAGS = -O3"; comment it by replacing it with "# OPTFLAGS = -O3". Go to $SME_Home/lib/SME. Open the file "tool_support". Comment two lines so that they read "# BUILDFLAGS = -O3" and "# DRIVER_CFLAGS = -O3".	When the time comes to build HNMD.cc, compilation of HNMD.o will exhaust virtual memory. Code optimization consumes the memory; so, one overcomes this obstacle by disabling code optimization in the SME program. One disables optimization by commenting lines of code that include "-O3" in two SME program files.
5.	Create a new project called hunt3 using "SME hunt3 $SME_Home/Projects	
6.	Cut and paste: All data from $SME_Home/Projects/HUNT/Data into $SME_Home/hunt4/Data DIN.eqns DOM.eqns ET.eqns GLOB.eqns HYD.eqns MAC.eqns PAR.eqns into $SME_Home/Projects/hunt4/Models directory GWater.cc GWater.h Opt.cc Opt.h SWater4.cc SWater4.h SWater.cc SWater.h UCode.cc UCode.h into the the $SME_Home/Projects/hunt4/UserCode directory. HNMD.conf into the $SME_Home/Projects/Config directory	
7.	Declare an SME model using "SME model HNMD"	
8.	Declare an SME scenario using "SME scen 1990"	
9.	Import the "*.eqns" files using "SME import DIN.eqns DOM.eqns ET.eqns GLOB.eqns HYD.eqns MAC.eqns	

	PAR.eqns"	
10.	Link the UserCode in the "HNMD.MML.config" file	
11.	Import the "*.eqns" files again	
12.	Build the model using "SME build"	
13.	Cut and paste all links into the "HNMD.conf" file.	
14.	Run the model using the command line interface or the java view server.	At this point, a number of error messages will almost certainly appear. Instead of discussing and resolving them as part of the 14th step, the resolution of each post-run error is handled as a separate step.
15.	Find the "Environment" file in $SME_Home/Projects/hunt3/Data. Open the file. Change the directories for the four variables.	While attempting to run the model, the system may not find the "StudyArea" map in a certain directory. To surmount this obstacle, one must follow the stated procedure and change the directories to match the correct directories.
16.	Find the "!*.pts" files such as "!Hunt_prcp.pts" and change the specified directories to the correct directories. For example, the SME may search for data in /Documents/SME/Projects/PLM_climate when it should be searching in /usr/share/sme2/Projects/PLM_climate.	The SME may be unable to open "timeseries" files in the /Documents/SME/Projects/PLM_climate directory. One must find and edit these files as outlined in the procedure box to the right. Besides "timeseries" files, the SME will have trouble with other files; the same solution might apply to many of these files.
17.	Take care while editing configuration files.	While attempting to run the Hunting Creek model, the SME may suffer a "segmentation fault". This is likely caused by an improperly configured "HNMD.conf" file. The configuration files are quite sensitive to variable labels (ex. pm(), ip(0.0), etcetera).
18.	Cut and paste	This step might work as an

	$SME_Home/Projects/HUNT/Config/HNMD.conf to $SME_Home/Projects/hunt3/Config	alternative to linking the "HNMD.conf" file by hand. It simply replaces the newly generated HNMD.conf file with one from the "Hunt.tar" file.

Appendix C:

Data Processing Algorithms Implemented in MATLAB

Appendix C contains the MATLAB algorithms used to process the data obtained during the experiments. The first section, Section C.1, holds the code for the main program. Each section after the first contains either necessary or optional subroutines found in the main program. The subroutines appear in the appendix in the order that they appear in the main program.

C.1 Main Program: Compare Arrays v4

As with most main programs, Compare Arrays v4 serves as the nexus for multiple subroutines. The main program contains function calls for all of the subroutines listed in Sections C.2-C.6. It is also the program with which the user is most likely to interact. The section labeled 'Visualizing Results' contains function calls for a number of internal MATLAB subroutines. A user is likely to utilize these one or more of these function calls extensively during a data analysis.

```
%Program Name: Compare Arrays v4
%****************************************************************************
%Description:
%This program automates the analysis of ASCII map files output by the SME.
%Specifically, the program compares map files and plots the results in
%various forms.  Version 4 improves program control by defining string
%variables; it does not offer more functions than version 3.

%Notes:  1.  The array with lower values should be entered first.
%        2.  If the computer designates a file as a "000000ASCII file,"
%              one must add ".000000ASCII" to the end of the file name.
%****************************************************************************

%Begin Program*****
%****************************************************************************
```

```
%Enter Directory Variables

baseline = '\Baseline'        %'Baseline' is needed for Water and 'Baseline_2' is needed for
WandBmass
scen_name = '\S_Water'   %Often is one of: G_Water, S_Water, GtoS_Water, WandBmass
location = '\Location_A'     %Is one of: Location_1-5 or Location_A-B
var_name = '\tot_npp'        %Often it is one of: din_sf, sat_water, surf_water, tot_npp

%Enter File Names and Dimensions
file_1 = ['c:\John_Reap\MS_Thesis\Scen_Data', baseline, '\Day_365\', var_name, '-
365.000000ASCII'];  %Baseline

file_2 = ['c:\John_Reap\MS_Thesis\Scen_Data', scen_name, location, '\Low', var_name, '-
365.000000ASCII'];
file_3 = ['c:\John_Reap\MS_Thesis\Scen_Data', scen_name, location, '\Med', var_name, '-
365.000000ASCII'];
file_4 = ['c:\John_Reap\MS_Thesis\Scen_Data', scen_name, location, '\High', var_name, '-
365.000000ASCII'];


rows=58;    %Size of the Hunting Creek spatial variables
cols=58;

%Importing, Translating and Cleaning Arrays
[array_1] = ASCII_trans_v2(file_1, rows, cols);
[array_2] = ASCII_trans_v2(file_2, rows, cols);
[array_3] = ASCII_trans_v2(file_3, rows, cols);
[array_4] = ASCII_trans_v2(file_4, rows, cols);

%Computing the Differences in the Arrays
array_diff_12 = array_2 - array_1;
array_diff_13 = array_3 - array_1;
array_diff_14 = array_4 - array_1;

%Array Derivation
[combined_array] = Combined_Ext_Map(array_diff_12, array_diff_13, array_diff_14, rows, cols);
[map_array] = Map_Maker(array_1, rows, cols);
ad_s = sparse(array_diff_13);


%Array Metric Calculation
[sum_A, count_A, avg_A, sum_B, count_B, avg_B, sum_C, count_C, avg_C] =
Avg_Array(array_diff_12, array_diff_13, array_diff_14, rows, cols);
sum_cells_vec = [sum_A; sum_B; sum_C]
affected_cell_vec = [count_A; count_B; count_C]
avg_vec = [avg_A; avg_B; avg_C]

%Preparing Arrays for Visualization Algorithms
[array_1_rev] = Column_Rev(array_1, rows, cols);          %Using the "Column_Rev" function to
prepare arrays
[array_4_rev] = Column_Rev(array_4, rows, cols);          %for the "surface()" function; the data
must be reversed.
[array_2_rev] = Column_Rev(array_2, rows, cols);
[array_3_rev] = Column_Rev(array_3, rows, cols);

[array_diff_12_rev] = Column_Rev(array_diff_12, rows, cols);
```

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```
[array_diff_13_rev] = Column_Rev(array_diff_13, rows, cols);
[array_diff_14_rev] = Column_Rev(array_diff_14, rows, cols);

[combined_array_rev] = Column_Rev(combined_array, rows, cols);
[map_array_rev] = Column_Rev(map_array, rows, cols);


%Visualizing Results

% 2-D Color-Coded Surface Plots
% figure, surface(array_1_rev)          %Provides a 2D plot of "spatial variable" - the map
% figure, surface(array_2_rev)
% figure, surface(array_3_rev)
% figure, surface(array_4_rev)

% figure, surface(array_diff_12_rev)
% figure, surface(array_diff_13_rev)
% figure, surface(array_diff_14_rev)

% figure, surface(map_array_rev)


% 3-D Surface Plots
% figure, meshz(array_4_rev)
% figure, meshz(array_diff_14_rev)

% figure, surf(array_2_rev)
% figure, surf(array_3_rev)
% figure, surf(array_4_rev)
% figure, surf(array_diff_12_rev)
% figure, surf(array_diff_13_rev)
% figure, surf(array_diff_14_rev)
%
% figure, surface(combined_array_rev)   %Plots differences between two maps


%Special Plots
% figure, spy(ad_s)                 %Plots geographic extent of the differences

% figure, contour(combined_array_rev)

% Adding Numerical Values to Contour Lines
% [C,h] = contour(array_diff_rev)
% clabel(C,h);
```

C.2 Translating Text Files into MATLAB Arrays

This critical subroutine translates raw spatial variable data from the SME into MATLAB arrays for further post-processing. One can use the code on any Hunting Creek spatial variable or other 58 by 58 spatial variable generated by the SME.

```
%Title: ASCII File Translator and "Cleaner"
```

```
%
%Description:
%This MATLAB program translates an ASCII text file output by a variant of
%the SME's Hunting Creek Model into a MATLAB array.  Then, it removes the
%excessively large dumby values from the imported array.  After completing
%these steps, the program outputs a MATLAB array that is ready for further
%post-processing.

function [array] = ASCII_trans(file, rows, cols)

[v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_9, v_10, v_11, v_12, v_13, v_14, v_15, v_16, v_17,
v_18, v_19, v_20, v_21, v_22, v_23, v_24, v_25, v_26, v_27, v_28, v_29, v_30, v_31, v_32, v_33,
v_34, v_35, v_36, v_37, v_38, v_39, v_40, v_41, v_42, v_43, v_44, v_45, v_46, v_47, v_48, v_49,
v_50, v_51, v_52, v_53, v_54, v_55, v_56, v_57, v_58] = textread(file,'%f %f %f %f %f %f %f %f
%f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f
%f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f %f', 'headerlines', 2);

%Initializing "array" variables:
n = 1;
m = 1;

% rows = 58;
% cols = 58;

% %file = 'Sat_waterB-365NoWell1'
% array = load(file)

array = [v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_9, v_10, v_11, v_12, v_13, v_14, v_15, v_16,
v_17, v_18, v_19, v_20, v_21, v_22, v_23, v_24, v_25, v_26, v_27, v_28, v_29, v_30, v_31, v_32,
v_33, v_34, v_35, v_36, v_37, v_38, v_39, v_40, v_41, v_42, v_43, v_44, v_45, v_46, v_47, v_48,
v_49, v_50, v_51, v_52, v_53, v_54, v_55, v_56, v_57, v_58];

while n < rows+1
while m < cols+1
if array(n,m)>1.00e+038
array(n,m)=0;
end
m=m+1;
end
m=1;
n=n+1;
end
```

C.3 Combining Maps for the Geographic Extent of Change

One of the functions of the main program is to calculate the difference between a
spatial variable from a baseline model and a spatial variable from a disturbed model.
Once calculated, this sub-program combines simplified versions of the difference arrays
for each of the three intensities. The resulting single array can later be further processed

to clearly reveal the different extents of the changes caused by the three disturbance

intensities.

```
%Title: Combining Extent Maps
%
%Description:
%This MATLAB program simplifies 3 input arrays and adds them.  Nonzero
%values in the first input array become 1s; values in the second become 2s.
%Values in the third become 3s.  The sum of the arrays is output.
%
%It provides a crude way of combining three difference arrays to illustrate
%the geographic extent of three design variable intensities simultaneously.

function [combined_array] = Comb_Ext_M(array_A, array_B, array_C, rows, cols)

%Initializing "array" variables:
n = 1;
m = 1;

% rows =3               %Test values
% cols =rows
%
% array_A=[0 0 .1; .1 0 0; .1 .1 0]
% array_B=[0 0 .2; 0 .2 0; .2 0 .2]
% array_C=[0 0 .3; 0 0 .3; 0 .3 .3]
%
% %[0 0 6; 1 2 3; 3 4 5]    %Expected result of test

while n < rows+1              % Sets nonzero cells to the appropriate
while m < cols+1          % value for each array
if array_A(n,m) ~= 0
array_A(n,m)=1;
end
if array_B(n,m) ~= 0
array_B(n,m)=2;
end
if array_C(n,m) ~= 0
array_C(n,m)=3;
end
m=m+1;
end
m=1;
n=n+1;
end

combined_array = array_A + array_B + array_C;
```

C.4 Extracting Maps for Display from the Data

The 'Map Maker' program does not function as a data processing algorithm. It exists to generate maps that highlight specific cells in the hunting creek watershed. Some of the thesis figures were created using this algorithm.

```
%Title: Map Maker
%
%Description:
%This MATLAB program creates arrays for display purposes.  It accepts
%a Hunting Creek array and converts it into a simplified array for
%display purposes.  Nonzero values are converted to 1s, and specific
%elements become 3s.  Elements with a value of 1 are set to 2.
%
%These arrays indicate the location of industrial disturbances.
%Note:  1) If a habitat map that indicates water as values of 1 is used,
%          this program will differentiate these locations.

function [map_array] = Map_Maker(array_A, rows, cols)

%Initializing "array" variables:
n = 1;
m = 1;

% rows =3                %Test values
% cols =rows
%
% array_A=[0 0 .1; .1 0 0; .1 .1 0]
%
% [1 1 .1; .1 1 1; .1 .1 1]    %Expected result of test

while n < rows+1            % Sets nonzero cells to the appropriate
while m < cols+1          % value for the array
if array_A(n,m) > 1    % Elements greater than 1 are set to 2
array_A(n,m)=2;
end
if n==26 && m==16      % Specific elements are set to 3
array_A(n,m)=3;
end
if n==31 && m==31
array_A(n,m)=3;
end
if n==36 && m==51
array_A(n,m)=3;
end
if n==33 && m==19
array_A(n,m)=3;
end
if n==33 && m==20
array_A(n,m)=3;
end
m=m+1;
```

```
end
m=1;
n=n+1;
end

map_array = array_A;
```

C.5 Calculating Metrics and Measures for the Difference Arrays

Given difference arrays calculated by the main program, the 'Averaging Arrays'

program calculates the metrics and measures seen in the results sections of Chapter 4.

```
%Title: Averaging Arrays
%
%Description:
%This MATLAB program calculates scalar averages for the contents of three input
%arrays.  It adds the the nonzero elements for each array and divides by the
%number of nonzero elements - thus producing an average.
%
%It provides a crude way of determining the magnitude of a control variable's
%impact on the landscape.

function [sum_A, count_A, avg_A, sum_B, count_B, avg_B, sum_C, count_C, avg_C] =
Avg_Array(array_A, array_B, array_C, rows, cols)

%Initializing "array" variables:
n = 1;
m = 1;

count_A = 0;
count_B = 0;
count_C = 0;

sum_A = 0;
sum_B = 0;
sum_C = 0;

cell_size = 40000;        %[m] size of one of Hunting Creek's cells

% rows =3              %Test values
% cols =rows
%
% array_A=[0 0 .1; .1 0 0; .1 .1 0]
% array_B=[0 0 .2; 0 .2 0; .2 0 .2]
% array_C=[0 0 .3; 0 0 .3; 0 .3 .3]
% %
% % .1, .2, .3    %Expected result of test

while n < rows+1            % Loops through the entire array
while m < cols+1
if array_A(n,m) ~= 0
sum_A = array_A(n,m) + sum_A;   %Sums nonzero cells
count_A = count_A + 1;        %Counts nonzero cells
```

```
end
if array_B(n,m) ~= 0
sum_B = array_B(n,m) + sum_B;
count_B = count_B + 1;
end
if array_C(n,m) ~= 0
sum_C = array_C(n,m) + sum_C;
count_C = count_C + 1;
end
m=m+1;
end
m=1;
n=n+1;
end

avg_A = sum_A/count_A;      %Divides cell sums by number of cells to get an average
avg_B = sum_B/count_B;
avg_C = sum_C/count_C;
```

C.6 Preparing Array Data for Display

A number of two and three dimensional MATLAB visualization functions consider the last element of the first column of an array to be element (1,1). Since this element is actually (1,n), one must reverse the columns of the arrays used in the main program before passing them to the MATLAB visualization functions. 'Column Reversing' accomplishes this important task.

```
%Title: Column Reversing
%
%Description:
%This MATLAB program reverses the row order in a matrix. For example, a matrix
%with rows 1, 2 and 3 would become a matrix with rows 3, 2 and 1. This
%program's primary purpose is to prepare arrays for plotting using MATLAB's
%"surface()" function.

function [array_rev] = Column_Rev(array, rows, cols)

%Initializing "array" variables:
n = 1;
m = 1;

while n < rows+1
while m < cols+1
array_rev((rows+1)-n,m)=array(n,m);
m=m+1;
end
m=1;
n=n+1;
end
```

REFERENCES

Abdel-Razik, M. (1989). "A Model of the Productivity of Olive Trees Under Optional Water and Nutrient Supply in Desert Conditions." *Ecological Modelling* 45: 179-204.

"About the WBCSD"(2003). World Business Council for Sustainable Development,

Allen, D.T. and D.R. Shonnard (2002). Green engineering: environmentally conscious design of chemical processes. Upper Saddle River, Prentice-Hall, Inc.

Askin, R.G. and C.R. Standridge (1993). Modeling and Analysis of Manufacturing Systems. New York, John Wiley & Sons, Inc.

Bailey, R., B. Bras and J. Allen (2001). "Measuring Material Cycling in Industrial Systems". IEEE Symposium on Electronics and the Environment, Denver, CO.

Bossel, H. and H. Krieger (1991). "Simulation model of natural tropical forest dynamics." *Ecological Modelling* 59: 37-71.

Boyce, W.E. and R.C. DiPrima (1997). Elementary Differential Equations and Boundary Value Problems. New York, John Wiley & Sons, Inc.

Butler, T.J., G.E. Likens, F.M. Vermeylen and B.J.B. Stunder (2003). "The relation between NO_x emissions and precipitation NO_3- in the easter USA." *Atmospheric Environment* 37: 2093-2104.

Cazelles, B., D. Fontvieille and N.P. Chau (1991). "Self-purification in a lotic ecosystem: a model of dissolved organic carbon and benthic microorganisms dynamics." *Ecological Modelling* 58: 91-117.

Cengel, Y.A. and M.A. Boles (1998). Thermodynamics: An Engineering Approach. Boston, McGraw-Hill.

Consoli, F., D. Allen, I. Boustead and J. Fava (1993). "Guidelines for Life-Cycle Assessment: A 'Code of Practice'". The SETAC Workshop, Sesimbra, Portugal, 31 March - 3 April, Society of Environmental Toxicology And Chemistry (SETAC).

Costanza, R., J. Cumberland, H. Daly, R. Goodland and R. Norgaard (1997). An Introduction to Ecological Economics. Boca Raton, St. Lucie Press.

Costanza, R., F.H. Sklar and M.L. White (1990). "Modeling Coastal Landscape Dynamics." *BioScience* 40(2): 91-107.

Costanza, R., A. Voinov, R. Boumans, T. Maxwell, F. Villa, L. Wainger and H. Voinov (2002). "Integrated Ecological Economic Modeling of the Patuxent River Watershed, Maryland." *Ecological Monographs* 72(2): 203-231.

DeAngelis, D.L., L. Godbout and B.J. Shuter (1991). "An individual-based approach to predicting density-dependent dynamics in smallmouth bass populations." *Ecological Modelling* 57: 91-115.

Elkington, J. (1998). Cannibals With Forks: the triple bottom line of 21st century business. Stony Creek, New Society Publishers.

Emblemsvåg, J. and B.A. Bras (2000). Activity-Based Cost and Environmental Management - A Different Approach to the ISO 14000 Compliance. Boston/Dordrecht/London, Kluwer Academic Publishers.

Epstein, M.J. and P.S. Wisner (2001). "Using a Balanced Scorecard to Implement Sustainability." *Environmental Quality Management* 11(2): 1-10.

Fisher, B.E.A., E. Metcalfe, I. Vince and A. Yates (2001). "Modelling plume rise and dispersion from pool fires." *Atmospheric Environment* 35: 2101-2110.

Fitz, H.C., E.B. DeBellevue, R. Costanza, R. Boumans, T. Maxwell, L. Wainger and F.H. Sklar (1996). "Development of a general ecosystem model for a range of scales and ecosystems." *Ecological Modelling* 88: 263-295.

Frosch, R.A., D.C. Bonner, J.B. Carberry, L. Carothers, D. Ditz, T.N. Gladwin, T.E. Graedel, C. Green, R.R. Gustafson, M.J. Leake, D.W. Mayer, R.D. Morgenstern, W.F. Powers and D.K. Williams (1999). Industrial Environmental Performance Metrics: Challenges and Opportunities. Washington, D.C., National Academy Press.

Galitsky, C., E. Worrel and M. Ruth, "Energy Efficiency Improvement and Cost Savings Opportunities for the Corn Wet Milling Industry," Technical Report LBNL-52307, July 2003.

Greiner, R. (2004). "Systems framework for regional-scale integrated modelling and assessment." *Mathematics and Computers in Simulation* 64(1): 41-51.

Hangos, K. and I. Cameron (2001). Process Modelling and Model Analysis. San Diego, Academic Press.

Hawken, P. (1993). The Ecology of Commerce. New York, Harper-Collins Publishers.

Hopp, J.W. and M.L. Spearman (1996). Factory Physics Foundations of Manufacturing Management. Chicago, Irwin.

Hudak, P.F. (1999). Principles of Hyrdogeology 2nd Edition. Boca Raton, Lewis Publishers.

Irving, J.M. "McNeil Generating Station, Burlington, Vermont". Burlington Electric Department, http://www.westbioenergy.org/lessons/les04.htm

Jorgensen, S.E., B. Halling-Sorensen and S.N. Nielson, Eds. (1996). Handbook of Environmental and Ecological Modeling. Boca Raton, Lewis Publishers.

Kalpakjian, S. (1997). Manufacturing Processes for Engineering Materials. Menlo Park, Addison-Wesley.

Leopold, A. (1948). The Land Ethic: 201-226.

Malanson, G.P., W.E. Westman and Y.-L.Y. Yan (1992). "Realized versus fundamental niche functions in a model of chaparral response to climate change." *Ecological Modelling* 64: 261-277.

Maxwell, T. (2002). "The Spatial Modeling Environment Users Guide". The Gund Institute for Ecological Economics, http://www.uvm.edu/giee/SME3/ftp/Docs/UsersGuide.html

Maxwell, T. (1995). Spatial Modeling Environment: README file in the SME distribution.

Maxwell, T. (1999). "A paris-model approach to modular simulation." *Environmental Modelling & Software* 14: 511-517.

Maxwell, T. and R. Costanza (1997). "A language for modular spatio-temporal simulation." *Ecological Modelling* 103: 105-113.

Maxwell, T. and A. Voinov (2004). "Spatial Modeling Environment". https://sourceforge.net/projects/smodenv/

Mclaughlin, S.B., D.G.d.l.T. Ugarte, C.T.J. Garten, L.R. Lynd, M.A. Sanderson, V.R. Tolbert and D.D. Wolf (2002). "High-Value Renewable Energy from Prairie Grasses." *Environmental Science & Technology* 36(10): 2122-2129.

Michaelis, L. (2003). "The role of business in sustainable consumption." *Journal of Cleaner Production* 11(8): 915-921.

Norton, B.G. and B. Hannon (1997). "Environmental Values: A Place-Based Theory." *Environmental Ethics*: 227-245.

Odum, E.P. (1987). Basic Ecology. Philadelphia, Saunders College Publishing.

O'Riordan, T. (1996). Democracy and the sustainability transition. Democracy and the Environment: Problems and Prospects. W. Lofferty and J. Meadowcroft. Cheltenham, Edward Elgan.

Pahl, G. and W. Beitz (1999). <u>Engineering Design A Systematic Approach</u>. London, Springer-Verlag.

Palacios, M., F. Kirchner, A. Martilli, A. Clappier, F. Martin and M.E. Rodriguez (2002). "Summer ozone episodes in the Greater Madrid area. Analyzing the ozone response to abatement strategies by modelling." *Atmospheric Environment* 36: 5323-5333.

Patterson, S. and D. Mackay (1989). "A Model Illustrating the Environmental Fate, Exposure and Human Uptake of Persistent Organic Chemicals." *Ecological Modelling* 47: 85-114.

Quazi, H.A. (2001). "Sustainable development: integrating enironmental issues into strategic planning." *Industrial Management & Data Systems* 101(2): 64-70.

Ramsey, S. (2002). "Measure environmental performance." *Pollution Engineering* 34(8): 28-30.

Reap, J.J., P.J. Newcomb, C. Carmichael and B. Bras (2003). "Improving Life Cycle Assessment by Including Spatial, Dynamic and Place-Based Modeling". Design Engineering Technical Conferences and Computers and Information in Engineering Conference, Chicago, Illinois USA, ASME.

Schmitz, R.J. (1996). <u>Introduction to Water Pollution Biology</u>. Houston, Gulf Publishing Company.

Schwarz, J., B. Beloff and E. Beaver (2002). "Use Sustainability Metrics to Guide Decision-Making." *Chemical Engineering Progress* 98(7): 58-63.

Seppelt, R. and A. Voinov (2002). "Optimization methodology for land use patterns using spatially explicit landscape models." *Ecological Modelling* 151: 125-142.

Simon, H. (2001). <u>The Sciences of the Artificial</u>. Cambridge, The MIT Press.

Solow, R.M. (1991). "Sustainability: An Economist's Perspective". J. Seward Johnson Lecture to the Marine Policy Center, Woods Hole, Massachusetts.

Turner, M.G., R.H. Gardner and R.V. O'Neill (2001). <u>Landscape Ecology in Theory and Practice: Pattern and Process</u>. New York, Springer-Verlag.

Voinov, A. (2004). "Re: Bugging the Master of the Model". J. J. Reap.

Voinov, A., R. Costanza, L. Wainger, R. Boumans, F. Villa, T. Maxwell and H. Voinov (1999a). "Patuxent landscape model: integrating ecological economic modeling of a watershed." *Environmental Modelling & Software* 14(5): 473-491.

Voinov, A., C. Fitz, T. Maxwell, R. Boumans and R. Costanza (2002). "Modular Ecosystem Modeling". IEMSS, Lugano, Switzerland.

Voinov, A. and H. Voinov (2003). "Library of Hydro-Ecological Models". Gund Institute for Ecological Economics at the University of Vermont, http://www.uvm.edu/giee/LHEM/

Voinov, A.A., H. Voinov and R. Costanza (1999b). "Surface water flow in landscape models: 2. Patuxent watershed case study." *Ecological Modelling* 119: 211-230.

Wackernagel, M. and W. Rees (1996). Our Ecological Footprint: Reducing Human Impact on the Earth. Gabriola Island, New Society Publishers.

Webster's New Universal Unabridged Dictionary Deluxe 2nd Edition (1972). New York, Simon and Schuster.