COMPUTATIONAL SUSTAINABILITY ASSESSMENT:

AGENT-BASED MODELS & AGRICULTURAL INDUSTRIAL ECOLOGY

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Executive Summary

Today, the vast majority of our industrial production systems is developed with linear assumptions. We extract natural resources, use them to produce goods and services and dispose the resulting wastes back into the environment. However, these processes have been contributing to serious environmental consequences and at the same time, important social costs. This PhD thesis analyzes the development of a methodological framework that aims at quantifying sustainability, using systems integration through a closed-loop approach in material and energy cycles for agriculture-based product on a regional context. The main objective of this research was to develop a decisionmaking tool that can help assess the sustainability of such systems, in part by reducing the overall consumption of energy and natural resources, and by improving the social, economic, and environmental performance of the network.

This research engages in the effort of promoting the concrete application of industrial ecology and takes human decisionmaking as a starting point in exploring underlying factors stimulating sustainable behavior. We applied our methodology that focuses on agricultural-based product industry in two regional case studies: the adoption factors that have specific impacts on switchgrass' life-cycle assessment (LCA) in the State of Michigan (USA), and the identification of the factors that promote the development of a regional industrial symbiosis in the Champagne-Ardenne region (France). Industry may provide an example on how a resource and/or waste can be managed to provide a sustainable supply chain to meet society's current and future needs in consumption. Yet biomass crop adoption and industrial symbiosis development are complex socio-technical phenomenon. Therefore, we built an agent-based model for each case study to describe the decision-making and the associated impact on the environment.

The computer-based practical implementation of this research was translated in the NetLogo software for two Agent-Based (AB) models. With regards to the first model, a hybrid AB-LCA approach had been chosen to better understand the main factors that influence decision-making and how adoption patterns can in turn affect the LCA of switchgrass ethanol. The second model is about the development of an Industrial Symbiosis (IS) at the regional scale. This AB-IS model focuses on the cultural and behavioral aspects, specifically on identifying levels of endogenous factors (cultural cooperation, social learning ability etc.) necessary for IS development and durability.

Both models have proved that they add meaningful value to building information modeling, which is currently lacking the human factor of decisionmaking. In the first AB-LCA model, the results show that the most influential factors affecting farmers' decisions are their current economic situation and crop prices. Age and their level of knowledge of the new crop have some impact but with more limited extent. It was shown as well that under similar allocations, ABM produced calculations that greatly varied from LCA calculations across different categories. In the second AB-IS model, the results showed that social learning has more impact on the positive development of the symbiosis than cultural cooperation. However cultural cooperation is needed in most situations in order to promote by-product exchanges when the simulation begins. This model revealed that individual social learning has an unambiguous downstream environmental impact over the network.

Keywords: Sustainable development, Industrial ecology, Life-cycle assessment, Distributed artificial intelligence, Agriculture, Biomass energy

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List of abbreviations

Abbreviation	Meaning
ABM	Agent-Based Model
ARD	Agro-industrie Recherches et Développement
CAS	Complex Adaptive System
CBA	Cost-Benefit Analysis
CCL	Center for Connected Learning
CE	Circular Economy
CLCA	Consequential Life Cycle Assessment
CREIDD	Research Centre for Environmental Studies and Sustainability
CRP	Conservation Reserve Program
EIA	Environmental Impact Assessment
EID	Eco-Industrial development
EIP	Eco-Industrial Park
EISA	Energy Independence and Security Act
EPD	Environmental Product Declaration
GHG	Greenhouse Gases
GE	Genetically Engineered
GIS	Geographic Information System
GPS	Global Positioning System
GREET	Greenhouse Gases Regulated Emissions and Energy Use in Transportation
GUI	Graphical User Interface
GWP	Global-Warming Potential
INES	INdustrial EcoSystem
ISO	International Standard Organization
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCSA	Life Cycle Sustainable Assessment
MCDA	Multi-Criteria Decision Analysis
MMT	Million Metric Ton
MWH	MegaWatt per Hour

PCSD	President's Council on Sustainable Development
RED-IBIS	Research for Envisioning Deliberate Integration of Biorefineries and Sustainability
RFS	The Renewable Fuels Standard
RPS	Renewables Portfolio Standard
SAS	Société par Action Simplifiée
SOHO	Self-Organizing Hierarchical Open
TBL	Triple Bottom line
TFC	Total Fixed Cost
UNEP	United Nations Environmental Program
USDA	United States Department of Agriculture
UTT	University of Technology of Troyes

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Chapter 1 Introduction and Theory

1.1 Introduction

Climate change is one of the six environmental challenges of the 21st century and is often cited as the ‘single greatest challenge facing decision makers on many levels’ [Ban 2009]. The transition to a low carbon society is one strategy to mitigate climate change. This includes energy generated from renewable energy sources, from, for example, biomass. Bioenergy replaces fossil fuelled energy and has the potential to decrease greenhouse gas emissions and to contribute to climate change mitigation. With its goal of 20% renewable energy by 2020 the EU pushes each member state for increased use of renewable energy [Directive 2009]. Today, most production systems continue to be developed from a linear thinking perspective - we extract natural resources, use them to produce goods and services, and then dispose the resulting wastes and emissions into the natural environment. However, such linear thinking-based productions have resulted to critical environmental and social consequences. In 1989, Frosch and Gallopoulos stated that one way to minimize these impacts could be to model our systems of production and consumption from an ecosystem-based inspired perspective [Frosch and Gallopoulos 1989]. The main objective behind their approach is to achieve industrial symbiosis by closing the loops: “The ultimate goal of industrial ecology is to reuse, repair, recover, remanufacture, or recycle products and by-products on a large scale” [Graedel and Allenby 2002]. Today, not only is the concept of industrial ecology rapidly evolving, but a practical application of it called Eco-Industrial Park (EIP), industrial ecosystem or network, has also emerged over the last thirty years.

In this thesis, we envision closing the loop by first, identifying the driving forces that promote the production of feedstock biomass and the increasing and the efficiency of natural resource consumption by closing the material and mineral cycles and implementing energy cascading by optimizing internal resource use and exchange. Closing loops also requires integrating industrial, economic, environmental and more importantly social systems with their behavioral believes that have been previously viewed as separate systems. This integration implies new interactions between various actors, each with its own motivations, which may have conflicting interests. Therefore, computational research is needed to study these interactions and their consequences in the environmental, economic and social realms [Bichraoui et al. 2013a]. The long-term goal of this project is to develop a tool that would help policy makers and industrial managers on possible industrial symbiosis implementation.

This thesis focuses on the development of a modeling approach for quantifying sustainability using a systems thinking approach using two case study that could potentially promote material and energy closing cycles for feedstock biomass products within a regional context. The first case study is seen as a way of testing this theorical concept by assessing the main factors that contribute to switchgrass adoption by farmers as a biomass feedstock, and its effect on its environmental life cycle using a hybrid agent-based (AB) and life cycle assessment (LCA) model. The second case study, takes AB modeling to the next level by combining Geographic Information System and an ABM and using actual material flow data form an industrial ecosystem. The goal of this model is to reveal the influential factors that favor symbiotic opportunities within the agricultural-based industry in Champagne-Ardenne (France). This can ultimately lead to a better understanding and unraveling of the dynamics of a complex system within an industrial ecosystem.

Overall, the main objective of this project is to show the development of a computational decision-making tool that can help in assessing the sustainability of such system by reducing the overall consumption of energy and natural resources and by improving the economic, environmental and social performance of the industrial network.

1.2 Motivation

In our introduction we have mentioned the world growing concern about the deteriorating condition of the environment and our common future has spurred research into the design of environmentally benign products and processes. As a result, localized actions and “end-of-pipe” solutions have recently been overtaken by approaches in which environmental issues are considered in the early design stages (i.e., Design For Environment). Therefore, as researchers we need to develop better metrics, indicators, assessment tools and more integrated predictive models to assist in evaluating engineering alternatives and management decisions. This research ambition to be part of the solution by providing a new system thinking perspective methodology that will make up for the weaknesses of existing disparate methods. These case studies will promote the development of dynamic models scenarios that will help us understand and therefore reduce the overall environmental and social impacts of activities within an industrial eco-system.

The chosen integrative computational approach will support the analysis of responses to changes in system behavior and check its robustness. This work is based on the industrial ecology approach in which the larger picture of an entire system is used to enhance the treatment of environmental concerns. More precisely, we proposed a modeling methodology that will support the understanding of an agricultural /industrial system for local context. Indeed, by modeling locally relevant variables, this methodology could be applied to different kinds of economic, social and environmental contexts, such as developing specific biomass adoption policies or implementing industrial ecosystem in developing countries. Moreover, implementing an industrial ecosystem using a holistic approach will enable the identification of critical but unseen linkages between actors that could have not been detected if investigated from a strictly linear or reductionist perspective. Identification of these inter-linkages could subsequently be used to influence public policy and affect structural changes at local, regional, and international levels.

Finally, implementing this integrative methodology within an eco-industrial system will require a shift in the current culture of researchers working at distributed sites with individual outcomes to a culture that includes the pooling of capabilities, sharing of information, materials, technology, and knowledge. This represents a new paradigm for traditional engineering research. Even though the role of specialized researchers will remain important in their respective fields, their findings will increasingly be applied across disciplines, and the relevance of their results will be valued as part of the whole. Moreover, the use of simulation modeling such as ABM for this type of project will provide broader insights on the potential of dynamic simulation modeling for large-scale projects on complex system that would otherwise require infrastructure use to test the feasibility of the model. In the next section, the scientific positioning and the integration of this thesis within the greater sustainability research realm, as well as the reason why we choose the proposed methodological framework is explained in greater detail.

1.3 Scientific relevance

As a PhD thesis, this project aims to advance and contribute to the realm of science. Here, we tried to impact the following fields of science: Computational sustainability, policy and management and the field of Industrial Ecology. Policy and Management deals with the difficult link between engineered physical systems and the policies that relate to this engineered system as well as the management of these techno-structure that use and depend on such systems. The view of the world is one of multi-agents systems. This research work aims to contribute by providing an approach to create computational models where these two aspects (physical and social) converge. Artificial intelligence is a broad research field, for which, the aim is to “understand” and “capture” human intelligence, learn from it and use it to create so called “knowledge based systems” [Sterelny 2007]. In this thesis AB modeling, a widely used approach from the field of artificial intelligence is applied to capture the socio-technical system. No fundamentally new developments are made that contribute to this scientific domain, but this thesis applies ontology in a novel way to setup AB models. By combining existing knowledge it contributes to this field of research. Existing knowledge is combined to create something new, but moreover new insights into how computational modeling paradigms differ from each other are presented. Traditionally, models of process systems are mostly approached through the physical aspects while the social and cognitive layer are often ignored. In this thesis, it is stated that the social elements such as behavioral believe, social learning and cooperation are not only critical but needs to be systematically included into sustainability-based models.

1.4 Goal and research question

As already stated, the focal point of this thesis is developing a general framework for simulating the sustainability of resource biomass use; this theme is analyzed here from a multi-agents modeling perspective. Although significant literature exists pertaining to the agent-based simulation of measuring environmental impacts, few studies have modeled the human behavior and its impact of its environment in general, with none simulating individual actions with the purpose of exploring a range of emergent behavior with its relationship to the natural environment. The exploitation of such model as the framework for the analysis was also one of the a priori objectives of the thesis. The modeling approach was deemed important in order to provide quantitative answers to sustainable biomass use issues. Understanding the impact of human behavior of such systems is important when attempting to measure sustainability. In both case studies, dynamic modeling has been employed in order to take into account the dynamics of the studied system and its feedbacks. Following from the scientific relevance and motivation of this thesis, a number of research questions are posed here that will be answered in this thesis. The broader research question is the following:

What is a suitable modeling approach for sustainable socio-technical systems that allows the user to make social and technical changes in industrial ecosystem and help decision makers to experiment prospective "what-if" scenarios in a dynamic, and evolving environment?

To help answer this main question, the sub-question are formulated:

- *What does a sustainable modeling approach for socio-technical systems that integrates socio-cognitive variables looks like?*

This questions will be further refined in Chapter 3 and 4 when presenting the case studies in greater details. In order to better understand the structure of this research project, the next section will give the reader an overview of the thesis structure, followed by a preliminary introduction to each case study.

1.5 Thesis outline

Chapter 2 presents the theoretical foundation of the thesis discussing: Industrial Ecology and its application as an eco-industrial park (EIP) and its linkage to the theorical philosophy of system thinking. Since EIP is seen as being a path to industrial sustainability, we will provide a knowledge map on sustainability assessment and tools. The chosen methodology of this thesis being computational sustainability, the field will be briefly introduced followed by its modeling tools.

Chapter 3 aims to present the industrial background being the biomass industry and the framework methodology used in this research.

Chapter 4 presents the ABM case studies and their results.

Chapter 5 establishes conclusions pertaining to research limitations, implications, and contributions

Appendix A and B detail the models specifications and component parts from the perspective of the model's Netlogo coding.

Appendix C and D provide the behavior space analysis results of both models

Finally appendix E presents a possible future extension for both models, which is the SD model of the Oilseed bio-refinery synergies programmed in Stella.

1.6 Cases studies

In order to test and develop a thorough analysis of our research questions, we needed a real-world bounded system in the chosen field of biomass cascading and energy feedstock. To do so, two regional case studies had been chosen: the switchgrass adoption by farmers in the State of Michigan (USA) and the development of a Regional Industrial Symbiosis in the Champagne-Ardenne region (France). These system boundaries provide a spatial system where data can be collected and used as inputs in the ABM, as well as practical canvas to test hypothesis by developing a conceptual framework that could assist policy makers and actors in these regions in identifying effective and efficient adaptation and mitigation measures and potential consequence scenarios.

1.6.1 Case Study # 1: The effects of Michigan farmers adoption Switchgrass as a feedstock biomass on its LCA

Increasing demand for the production of energy from renewable sources has fueled a search for alternatives to supplement those currently in production. One such alternative is switchgrass, a perennial grass native to North America that appears to have considerable potential as a biomass feedstock for energy production. While the properties of switchgrass as a biomass feedstock have been intensively studied, the adoption pathways and the environmental impacts of these pathways have received much less attention

This study aims to understand the main factors influencing their decision-making and how these adoption patterns can affect the LCA of switchgrass ethanol. To help address these challenges, we developed an ABM aimed at:

1. Understanding the main factors influencing their decision-making and how these adoption patterns can affect the LCA of switchgrass ethanol and
2. Help improving the LCA modeling methodology by overcoming the issues involved with analyzing emerging technologies with dynamic and evolving supply chains and expanding the methodology to fit a sustainable framework.

1.6.2 Case Study # 2: The Champagne-Ardenne agriculture products industry as a Dynamic industrial eco-System

Industrial sustainability at the regional level requires collaborative efforts from various participating agents toward common goals consisting of resource conservation, low carbon emissions, production efficiency, economic viability, and corporate social responsibility [Bichraoui et al. 2013a]. This study is the follow-up work of the more advanced and improved version of the framework model previously developed by Bichraoui and al. [Bichraoui et al. 2013b]. This project aims to materialize the notion of systems sustainability by developing a combined Agent-Based (ABM) and Geographic Information System (GIS) model for the development of a potential industrial symbiosis. This model is part of case study exploring at the development of regional industrial symbiosis around the agricultural-based product industry in the Champagne-Ardenne region (France). In this thesis, we view these economic activities along with their associated partners (suppliers, customers, government agencies, etc.) and the natural environment in which they operate as Complex Adaptive Systems (CAS). This task will help identify and provide a contextual analysis of structural factors and main driving forces for the development of a regional industrial symbiosis along the lines of prospective scenarios (ecological constraints; regulations, economic, cultural and behavioral contexts; carbon markets; technological routes; etc.).

By using ABM, social interaction and iteration are added to this framework, thus allowing for exploration of the role of industrial symbiosis development patterns. The model is to be used to get the following research insights:

1. Contribution to the development of models scenarios that will help us understand and therefore reduce the overall environmental and social impacts of activities within an industrial eco-system.
2. Helps foresee outcomes of change, and leads to improve management of coupled industrial/ecological systems by controlling anthropogenic activities

Chapter 2 Theoretical research foundations

2.1 Industrial Ecology

The famous Agenda 21 revealed during the Rio conference in 1992 is a process aiming at facilitating sustainable development at community level, whose participatory approach encompasses the social, cultural, economic and environmental needs of the present and future citizens [Summit 1992]. Industrial Ecology (IE) is a natural continuation of these elements; it is a cooperative approach to environmentally sustainable economic development and business-environment related issues

The concept of IE has roots back to the 1950's from a concern of potential limits of raw materials, caused by an increasing demand for resources. This area would later be termed as "industrial metabolism" [Ayres 1989]. In a special issue of Scientific American on "Managing planet earth", the core principles of IE were introduced to the scientific literature at large [Frosch and Gallopoulos 1989]. The notion of "industrial ecosystem", using the ecosystems in nature as models for the organization of industrial activity, was launched: "Wastes from one industrial process can serve as the raw material for another, thereby reducing the impact of industry on the environment" [Frosch and Gallopoulos 1989]. An other definition of IE is: "Industrial Ecology is the study of the flows of materials and energy in industrial and consumer activities, of the effect of these flows on the environment, and of the influence of economic, political, regulatory and social factors on the flow, use and transformation of resources" [White et al. 1994]. In short, industrial ecologists view industries as webs of producers, consumers and recyclers, and they encourage symbiotic relationships between companies and industries. The "ultimate goal of IE is to reuse, repair, recover, remanufacture, or recycle products and by-products on a very large scale" [Allenby 1994; Ayres and Ayres 1996; Frosch and Gallopoulos 1989; Garner and Keoleian 1995; Graedel and Allenby 2002]. Resource sharing among firms provides the potential to increase stability of operations, especially in supply-constrained areas by ensuring access to critical inputs such as water, energy, infrastructure and natural resources [Bichraoui et al. 2013a]. Today, not only the concept of IE is rapidly evolving, but a practical application of it, called Eco-Industrial Park (EIP), Industrial Symbiosis (IS) or network has emerged over the last thirty years. EIP concept and example of applications will be further presented in the next section.

2.1.1 Evolutionary approaches for the development of IS networks

Chertow [2000] states that successful industrial symbiosis endeavors are developed organically over time, and while there are ways to accelerate this process, an organic evolutionary approach is best when trying to move forward with industrial symbiosis projects. She describes three approaches to facilitate self-organized IS development which are presented below.

Existing by-product synergies

There are many examples of single by-product synergies. If one or more of these are identified and recognized for its economic value, the management of companies can be attracted to IS and understand that these synergies are not particularly risky or novel [Chertow 2000]. The single exchange can then be used as a catalyst to push for more exchanges and which could result in a working IS initiatives over time.

Existing organizational relationships

Existing organizational relationships or networks can be a nest for the birth of IS activities. Chertow [2000] mentions the textbook case of Kalundborg where an organization was formed to deal with the common problem of water scarcity and later became the source of ideas for other symbiotic relationships.

Anchor tenant model

The anchor tenant model suggests that one or two large industries with large input and output quantities can be the main actor and drive the network and attract other industries to join the industrial ecosystem [Chertow 2000]. Power plants are typical anchor tenants since they often can utilize a range of different fuels and provide many different products to a diverse range of customers. An institutional anchor tenant has been defined by Baas [1998], Korhonen et al [1999], Brand and de Bruijn [1999] and Mirata [2005] as a managing actor that oversees the system and provides with education, information, social and economic infrastructure and a discussion forum needed to maintain the "big picture" of the initiatives and promote its development.

Mirata [2005] found that institutional anchor tenants are as important as the other actors. He also found a Swedish IS network developed without a physical anchor tenant, but with the municipality's environmental department serving as an institutional anchor tenant with strong relationships to local industry.

2.1.2 Industrial ecology in practice: Eco-Industrial Park (EIP)

Literature on industrial eco-park is sporadic and not very dense despite a growing interest among scientists and eco-professionals. Eco-industrial development refers to a wide set of ideas and disciplines, and has been evolving over the years [Agarwal and Strachan 2006].

An EIP is:

- "A community of manufacturing and services businesses,
- Seeking enhanced environmental and economic performances,
- Through collaboration in managing environmental and resource issues
- Including flows of energy water and materials".

By working together, this community seeks a collective benefit that is greater than the sum of the separate benefits that each entities would make by optimizing its individual performance only [Flood 1999; Côté 2000].

Application of IE as a concrete industrial system implies the involvement of certain conditions, in her article "Uncovering Industrial Symbiosis", Chertow [2007] describes Industrial symbiosis as being characterized by a series of interrelationships between participating businesses such as:

- "Exchanges of material and energy among several firms within the network
- Waste exchanges initiatives between two or more firms
- LCA of all materials used by each facility or company
- Possibility of expanding the network toward a virtual ecosystem in which networking of various types occurs over a larger area."

On the other hand, Côté et.al [1998] who were among the first researchers to investigate industrial parks as ecosystems, emphasize the ecosystemic approach as the ultimate goal to reach in order to become a functioning industrial eco-park. According to Côté et.al [1998] industrial eco-park should achieve the following objectives:

- “The industrial activity take into account the ecological capacity of the area, in order to sustain industrial activity, focusing on the capacity of the environment (air, water and soil) to absorb emissions
- The energy production should be based on renewable resources and at least increase the efficiency of current energy production and use through cogeneration and district heating
- Buildings should be designed and built to optimize conservation of heat and water.
- Plants should be selected based in part on their potential for symbiosis
- The management of the network should involve not only producers and consumers but scavengers and decomposers to support recycling of materials
- Dissipative uses of materials and energy should be discouraged”.

Ehrenfeld and Gertler [1997] reviewed several emerging EIP and stated that the key factors of success are:

- “A strong regulatory framework that allows flexibility
- A continuous technical improvement, and community participation
- A flexible financing and taxes system that promote the reduction of waste and enhanced efficiency
- A transportation logistics system that encourages efficiency and sharing of facilities; sharing of information on operations especially on products and byproducts; and a diversity of small, medium and large industries.”

From a concept perspective, Agarwal and Strachan [2006] identified four types of conceptual eco-industrial development “that are considered to be the most relevant for the planning area in the US context:

• Eco-Park (Planned Mixed-Use Commercial Park): It would be branded and marketed as an eco-industrial park (EIP) and planned according to eco-industrial development principles including business-to-business and business-to-community networking, energy and resource efficiency, pollution prevention, sustainable land use and building design etc.;
• Bio-Based Industry Cluster: It would produce alternative fuels, lubricants and co-products increasing the value of agricultural resources such as corn and soybean (e.g. Biodiesel from soybean oil);
• High Performance Warehouse and Distribution Centers: It would be used for logistics division of retailers and wholesalers by co-locating combination of firms with complementary distribution channels;
• Research and Technology Park: focusing on commercialization of research"

Chertow [2003] categorized "eco-industrial development based on size and geographical coverage of its activities:

- Through waste exchanges, meaning that plants are recycling or selling recovered materials to other plants.
- Among firms co-located in an eco-industrial park, plants located in a defined geographical area exchange energy and material, share information and mutualize services such as transportation.
- Among local firms that are not collated, which relies on using existing businesses and attracting new ones to create to physically or virtually join the EIP".

According to the definitions of EIP development initiatives in the reviewed literature, we note that, although most of the definitions include the concept of IS the definition of EIP development has not yet set precise boundaries in order to identify what kind of initiatives can constitute an EIP development initiative [Agarwal and Strachan 2006]. In spite of the common use of the expression "eco-industrial parks", it is essential to note that industrial symbiotic relationships do not necessarily exist within the confines of a park [Harper and Graedel 2004]. In this thesis, EIP is considered to be a subset of IS by being a practical approach to achieve sustainable development.

2.1.2.1 Eco-industrial parks in development

Besides the level of coordination among participants, a major difference among the different EIPs is the degree to which participants are situated on the same site. For example, Brownsville, Texas, is developing one type of EIP, the “virtual” eco-industrial park, which is an affiliation or network of related regional companies. Although they are not physically located in the same park, by collaborating together, companies in a virtual park can create economies of scale. For instance, they can cooperatively buy goods with a higher recycled content, or hire a shared engineering efficiency expert or compliance auditor. Affiliated companies participating in waste exchange will pay lower prices for secondary raw materials and realize savings in hazardous waste disposal charges. For example, Mobil sells styrene/ethylbenzene for 50 cents to a recycler, whereas it used to cost $1 per gallon to dispose of it. In addition, clustered companies that are co-located in the same region can enjoy reduced transportation costs, whether the firms are industrial, commercial or retail establishments.

In Virginia, the Port of Cape Charles has developed a second type of park, the “zero-emissions eco-industrial park” [PCSD 1996]. The project‘s design is the most ambitious type of EIP, having a goal of the total elimination of emissions. Just as with the virtual EIP, participants receive a certain level of resource efficiency through cooperative buying, waste exchange, and so forth.

Another early example that engineered the byproduct-synergy concept was developed by Chaparral Steel in Texas. This industrial network involves a steel mill, a cement plant, and a car-shredding company. This project’s venture has been successful by not only reducing its costs and environmental impacts associated with the three companies but also by creating new opportunities including a patented process which is being marketed [PCSD 1996].

There is a growing interest in North America about EIP's. They are seen as an important element in any sustainable development strategy. No community in the United States has what can be called a functioning EIP. There are few examples worldwide, the most famous and documented Kalundborg, Denmark is described in greater details below.

The symbiosis of Kalundborg

There are many examples of symbioses and synergies described in the academic, technical, and Internet literature. The most famous eco-industrial park initiatives is the Kalundborg industrial symbiosis in Denmark in which 24 different symbioses have been explored over a 30-year period [Cuff and Goudie 2009]. This evolution has been particularly successful, both economically and environmentally [Ehrenfeld and Gertler 1997; Jacobsen 2006]. For this reason, Kalundborg has served as a model that many other industrial areas have attempted to emulate [Cuff and Goudie 2009].The first partners in kalundborg, an oil refinery, power station, gypsum board facility, pharmaceutical plant, and the city of Kalundborg, share ground water, surface water and waste water, steam and electricity, and also a variety of residues that become feedstock in other processes. The waste exchanges alone amount to some 2.9 millions tons of material per year; water consumption has been reduced by a collective 25%, and 5000 homes receive district heat [Chertow 2000] (see Figure 1). Cooperation has significantly increased environmental and economic efficiency, and at the same time has created many less tangible benefits for these industries, involving personal, equipment, and information sharing [J. Christensen 2007].

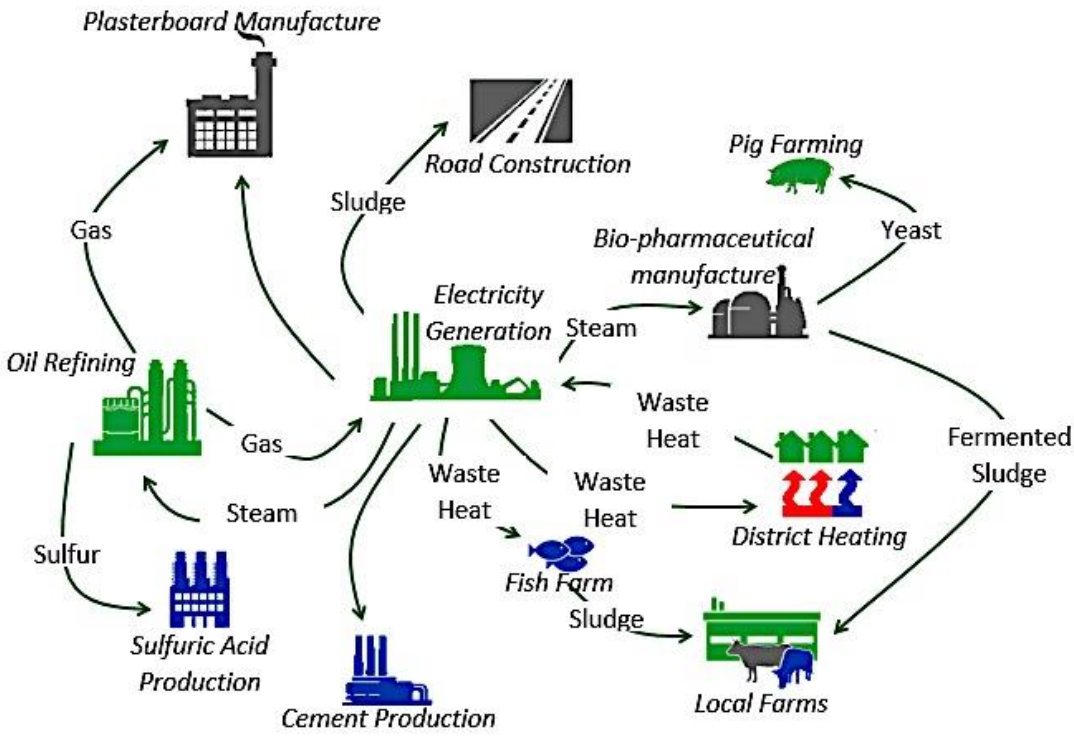


Figure 1: Kalundborg's industrial symbiosis diagram
Retrieved from http://www.energenz.com.hk/themes/circular-economy/industrial-symbiosis/

Clearly, IE is an ambitious field of study, however, some evolution such as providing tools quantifying EIP overall sustainability must still occur. Consequently, industrial networks have been the subject of many analyses and quantitative tools such as LCA and ABM, to analyze "industrial metabolism" [Suh 2004; Halog et al. 2011; Halog and Manik 2011]. These tools, some of which will be further presented in the next section, are steady-state tools and provide us with a snapshot of the system, whether it is a unit process, a plant, or a region. In this way, quantifying environmental and economic benefits is not only possible thanks to these exiting tools but also well established. However, measuring sustainability within industrial eco-system taking into account ecological and economic aspects but also social dimensions is still a remaining task, especially when this type of system is characterized as dynamic (over space and time) and complex (multitude of actors with a variety of interests and access to information) [Côté 2000]. In the next section we will discuss how sustainability assessment is addressed in the literature as well as how complexity and dynamics can be dealt with throughout computational sustainability methods.

2.1.3 Measuring environmental benefits of Industrial Symbiosis

We presented in the previous sections EIPs and how they work together, now we are focusing on how we can measure the environmental benefits of this type of eco-system. The by-product synergies linked to industrial symbiosis are often assumed to provide environmental benefits, contributing to the overall goal of sustainability that IE aims to achieve. Also, financial benefits are assumed to be achieved, describing industrial symbiosis as a "win-win" situation [Wolf 2007]. However, the lack of studies in the field confirming this theory is obvious. Very few attempts have been made to quantify these benefits, either theoretically or through case studies, and many of the existing studies often present neither assumptions nor methods for calculations.

Brings Jacobsen [2006] made a quantitative evaluation of parts of the Kalundborg industrial symbiosis system, but limited to a single resource - the water exchanges, and found some support for the theories of economic motivation as well as some environmental benefits. Some estimation of savings in water, oil equivalents and natural gypsum have also been made for the Kalundborg IS network [J. Christensen 2007] but these are typically presented without accounting for assumptions or the method of calculations. Singh et al. [2006] performed an LCA-type environmental impact assessment for different design schemes of an industrial ecosystem using a software tool. However, the different design schemes used include different plants and processes as well as new products, which make it difficult to see to what extent the environmental benefits can be attributed to IS in particular.

Industrial Ecologists try to analyze societal issues and their relationship with both socio-economic systems and the environment. Through this holistic view, researcher in IE recognize that solving problems must involve understanding the connections that exist between these systems, various aspects cannot be viewed in isolation [Halog and Manik 2011]. Often changes in one part of the system can spread and cause changes in another part of the system. Therefore, one can only solve a problem by dealing with at its parts in relation to the whole. Based on this framework, IE looks at environmental issues with a system thinking approach. Moreover, the systems IE has to deals with are complex systems. In order to understand this complexity, methodological modeling tools can be incorporated. The purpose of these tools is to help to identify those potential elements of an industrial ecosystem that could work together to achieve more eco-efficient outcomes [Batten 2009]. Computational sustainability modeling is a way of solving this kind of issues. Sustainability assessment tools and well as computational simulation tool and its framework will be further discussed in this chapter.

2.2 Quantifying Sustainability

Sustainable development was first introduced by the Brundtland Commission in 1987: as ‘‘development that meets the needs of the present without compromising the ability of future generations to meet their own needs’’ [Brundtland and others 1987] . Since the Brundtland Commission, this definition has been refined, and gave birth to the widely known “three pillars” or “triple bottom line” (TBL) of sustainable development introduced at the 2005 “World Summit” [Assembly 2005]. Generally, these indicators are either used in isolation to analyze the performance of sites, companies and sectors as they relate to one of the three dimensions, or, increasingly, in combination as a means of measuring progress towards and away from sustainability [Warhurst 2002]. In this thesis, these pillars are considered to be of equal importance. Therefore, in order to assess sustainability we need a set of tool that addresses these dimensions simultaneously. In the next section, we will present them separately but it is important to note that they are all interconnected; we will present later in this thesis how to deal and measure the consequences of these interactions.

2.2.1 Economic assessment

Although sustainability narrative has often been used to challenge traditional economic thinking, the economic approach as being part of sustainability has been tackled by various authors such as: Mäler [2008], Pezzey and Toman [2012] and Hamilton and Atkinson [2006]. Early contributions to the contemporary employed basic concepts concerning economic assets and sustainability, for example, Solow [1986] and the pioneering asset accounting study of Repetto et al. [1989] According to Hackler [2011] sustainable economic development is “pro-growth but concerned with equitable distribution and environmental awareness”. The philosophy behind these contributions is to develop a more inclusive approach in economic asset development that goes beyond more profitability.

A wide range of tools exist for economic assessment, they mainly consist of evaluating cost and profitability applied usually during process development; This steps has been summarized by Heinzle et. al. [2007] they basically include a series of estimations: The estimation of the capital investment based on the cost of equipment necessary (to operate a process), followed by the operating cost based on the cost of raw material, energy, labor etc. “Profitability analysis” evaluates the expected revenues and ranges them in proportion to the costs and to other factors such as “time-value” of money. Cost-benefit analysis (CBA) is a well-documented tool for assessing the net economic effects of policies metric [US EPA n.d.]. The focus of a CBA is a comparison of trade-offs: the total value of the benefits, in both demand and social objectives met, must exceed the opportunity cost of the consumed resources [Beria et al. 2012]. The relationship of CBA and with sustainability assessment is that the benefits of a project to society should not exceed the opportunity cost of using those resources elsewhere. Multi-criteria decision analysis (MCDA) is a tool for determining an optimal option from a limited set of options, when significant environmental, social and economic impacts need to be taken into account [Beria et al. 2012]. MCDA is intended to support the decision makers’ learning with respect to problem nature, existing priorities and preferences, values, and objectives and to lead them to a preferred option through synthesis, and application of models and methods [Omann 2004].The benefit of multi-criteria analysis in assessing the sustainable scenario is that it allows the use of both qualitative and quantitative criteria [Milutinović et al. 2014].

These tools were first developed to assess process sustainability but it seems that they could be expanded and then used to assess an eco-park sustainability for example the capital investment can measure the cost of shared facilities or equipment such as common transportation means. On the other hand, the profitability analysis could be used to assess the cost and benefits of potential synergies, for example calculating the potential gain in investing on waste exchange initiatives within an industrial ecosystem. The combination of this economic assessment tools could ultimately lead to answer questions about the success (or not) of the industrial ecosystem, the following questions had been developed by Chertow [2003]:

> "- Is the development commercially viable or does it requires outside subsidy? Often the public sector serves a catalytic role in Eco-Industrial development (EID), but after a defined time, a project will not be sustainable if it is significantly dependent on such subsidies.
>
> - Is the EID project structure more or less costly than conventional methods? Analysis concerning costs must be performed but should also include monetization of environmental benefits".

2.2.2 Environmental assessment

Gibson [2001] states that ''environmental assessment processes...are among the most promising venues for application of sustainability-based criteria. They "are forward looking, integrative, often flexible, and generally intended to force attention to otherwise neglected considerations'', although he also recognizes that ''environmental assessments are not the only vehicles for specifying sustainability principles, objectives and criteria'' [Gibson 2001].

The environmental benefits of an industrial ecosystem are quantified by measuring the changes in consumption of natural resources, and in emissions to air and water, through increased cycling of material and energy [Chertow 2007]. If we go back to the most famous industrial symbiosis achievement: Kalundborg, we can grasp the idea of how environmental and economic benefits might look like. A coal-fired electrical plant, an oil refinery, and other companies and manufacturers work together with the city of Kalundborg to effectively reduce consumption of resources and minimize waste. Kalundborg's industrial symbiosis yields significant reduction in oil, coal and water consumption as well as reducing carbon dioxide and sulfur dioxide emissions. While the initial investment was approximately $75 million, the partners estimated in 1999 that they had "saved" $160 million, making the average payback of an industrial symbiosis project like Kalundborg less than 5 years [Erkman 2001].

From a network perspective, recent efforts have been made in order to increase the availability of information, regarding the implementation and the development of industrial eco-park. A MediaWiki platform is in development, a website providing a worldwide database of Industrial eco-park site as well as a set of definition and evaluation criteria's such as: number of industrial sector involved, physical and social exchange with the community, resources exchange (water, energy, material, by-products), shared infrastructure and information within the eco-park, and benefits gained from the symbiosis (environmental, social ex: job creation). The goal of this platform is to bring together actors such as academic researchers and industrial actors, and policy makers that could be interested in the concept but usually do not communicate with each other [Wouters, S., and N. Feldmar. 2010].

When it comes to determining potential synergies from a spatial perspective, advances have also been made using geographical analysis. Virtual globe such as "Google Earth" is seen as a promising interface tool in order to "identify and quantify opportunities for materials and energy efficiency improvements", it has been tested in Pennsylvania, where data from the Department of Environmental Protection provided information about "the location of disposal and type of residual waste from sources producing more than one ton per month" According to Doyle and Pearce [Doyle and Pearce 2009]. The main findings of this investigation are that virtual globes coupled with open source waste information can be used to help:

- "Reduce embodied transport energy by reducing distances to recycling facilities,
- Choose end of life at recycling facilities rather than landfills, and
- Establish industrial symbiosis and eco-industrial parks on known by-product synergies".

The use of Open source information sharing seems to be useful in identifying economically and environmentally synergies for waste management if the data is available [Doyle and Pearce 2009].

LCA is a technique to assess the potential environmental impacts associated with a product or service throughout its life cycle [ISO 2006] ; i.e.: from raw materials through materials processing, manufacture, distribution, use, repair and maintenance, and disposal or recycling. The main categories of environmental impacts included in commercial LCA software tools are resource depletion, human toxicity, and ecological impacts. Performing an LCA can help in achieving a comprehensive outlook on the main environmental concerns for a product system and how to address them. In order to complete this type of study the following steps are necessary:

1. "Compiling an inventory of relevant energy and material inputs and environmental releases;
2. Evaluating the potential impacts associated with identified inputs and releases;
3. Interpreting the results to help you make a more informed decision" [ISO 2006].

Examples of environmental impacts categories are resource depletion (energy use and materials, land, and water), human health (toxicological impacts, and non-toxicological impacts), and ecological impact (acidification, ozone depletion, eutrophication, and global warming) [Lindfors 1995].

The application of the process, and associated waste minimization practices by management, design, and manufacturing can also lead to better and less polluting products that are less expensive and provide a marketing edge over the competition [ISO 2006] Figure 2 shows the LCA framework based on ISO 14040.

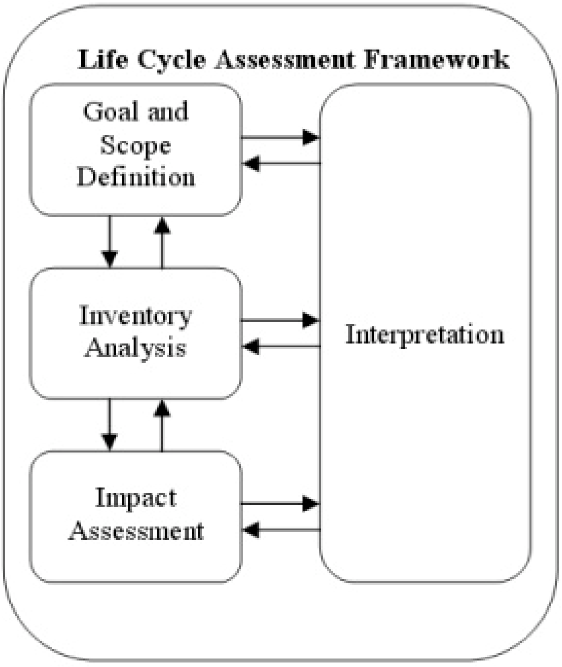


Figure 2: LCA framework [ISO 2006]

A life cycle of a product or a service starts with raw materials extraction, then production process and extended to use, transport, and disposal. LCA is "a technique for assessing the environmental aspects and potential impacts associated with a product, process, or system by:

- Compiling an inventory of inputs / outputs
- Evaluating potential impacts of those
- Interpreting result of the inventory and impact assessment in context of study objectives
- Suggesting improvements for future benefit" [ISO 2006]

There are two types of LCA: attributional and consequential. Attributional LCA describes all the pollution and resources flows within a defined system for a specific amount of the functional unit. The goal is to assess the total environmental burden. A consequential LCA, looks at estimating how pollution and resources flow within a defined system change in response to a change in demand [Thomassen et al. 2008]. The choice between both methods depends on the stated goal of the study [Curran et al. 2005]. Consequential LCA is still new in the field of study and therefore the least used.

From a company perspective, LCA study can assist in identifying improvement opportunities for product or its process, and identifying marketing opportunities by using LCA for eco-labeling, environmental product declaration (EPD) etc. From an industrial ecosystem perspective, consequential LCA can be used to assess the potential environmental impacts of a product system in response to a change in situation; for example what would be the potential environmental impact of the product system A, if the plant joins an industrial eco-park and replaces its input raw material by new by-products provided by waste from an other plant? What could be the social impact of such change in production? LCA cannot provide a complete answer because it's mainly based on assessing environmental impacts, however the results of such LCA can be estimated within a dynamic model, system dynamics for example, and then provide insights regarding social and economical impacts. This method can be applied each time a new synergy between two actors is considered. This will then help make a decision about whether to adopt this new synergy or not.

2.2.3 Social assessment

Another area of sustainable assessment issue is social assessment. Out of all three other pillars, it is still the least developed. Indeed as opposed to the previous aspects it lacks a broad consensus on adequate indicators or a standardized method of their identification (Halog & Manik, 2011). In order to address these challenges The Research Group for "Sustainable Production and Consumption" (SCP) has developed a social evaluation model of process /production in the biotechnology sector. It is intended to be used by companies for assessing potential sustainability risks and opportunities of biotechnological production. It resulted in identifying eight indicators for social assessment: "health and safety, quality of working conditions, impact on employment, education and training, knowledge management, innovative potential, customer acceptance and societal product benefit, and social dialogue" (Geibler & Al. 2006). These indicators had been identified through a survey of international stakeholders such as NGO's, unions, industries, academia, financial institutions, customers etc. Their focus was on discovering the relevant social aspect throughout the process/product life cycle. As for the economical assessment presented earlier, these indicators can be used in order to assess the overall social benefit of an industrial ecosystem, such assessment can answer questions like: Are the synergies beneficial to the community? Do they have more or a better access to “clean energy”, Does the economical savings from the applied synergies can create jobs? These questions might be difficult to answer just by performing linear assessment. Indeed, the participant actors from all dimensions (economical, social and environmental) interact with each other, each one of them bearing different interest and individual pattern of behavior, these nonlinear interactions give rise to emergent behavior (Rocha, 1999; Halog & Manik, 2011) which is today, commonly understood as the typical characteristic of a complex system.

Therefore, to understand the complexity, advanced methodological modeling tools should be developed. The purpose of these tools is to help identify those potential elements of an industrial ecosystem that could work in symbiosis to achieve more economically, socially and environmentally efficient outcomes. Here, modeling is seen as a way of solving problems that occurs in the “real world” which is used when creating a prototype or experimenting is impossible or too expensive (Ford, 1999; Halog & Manik, 2011). Our focus in this thesis is to demonstrate how simulation modeling method can be used and then combined in order to yield to a holistic assessment methodology for an industrial ecosystem. In the following section the concept of computational sustainability, as the focus of the research project, will be introduced as well as dynamic simulation tools such as systems dynamics and agent based modeling.

2.3 Computational Sustainability

Computational Sustainability is a new emerging research field with the overall goal of studying and providing solutions to computational problems for balancing environmental, economic, and societal needs for a sustainable future. The objective of this discipline is to develop computational and, mathematical models and methods for decision making concerning the management of natural resources in order to help address some of the challenging problems related to sustainability [Halog and Manik 2011]. Figure 3 shows the possible areas and interactions in computational sustainability.

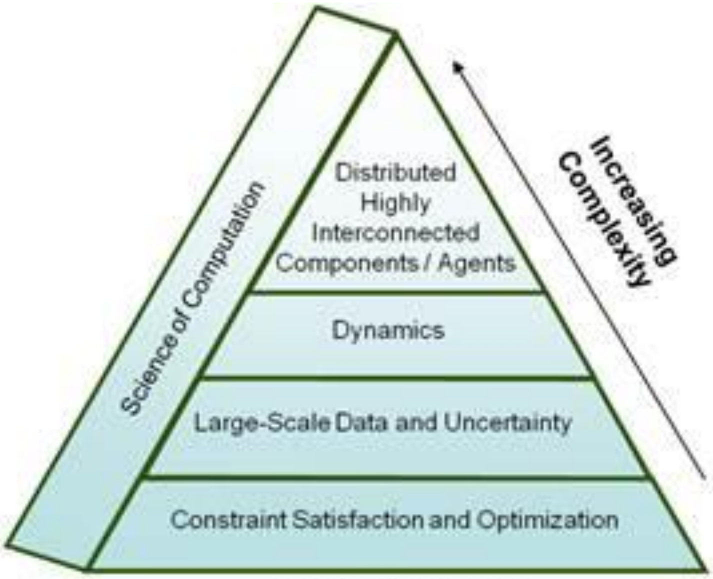


Figure 3: Research themes in computational sustainability [Institute for computational sustainability. Cornell University n.d.]

Making such decisions optimally present significant computational challenges that will require the efforts of researchers in computing, information science and related discipline. One way to answer these challenges is to create a methodological framework that can simultaneously integrate the three pillars of sustainability (social, environmental, economic) and has the ability to deal with the complexity of industrial eco-system in combined dynamic simulation modeling. In a complex system, where global behavior emerges from the complexity of micro-level behavior, which influences the macro-level, dynamic modeling allows the computation of micro and macro–level variables simultaneously. This tool offers a great opportunity to investigate numerous scenarios.

2.3.1 Organizational learning

Organizational learning is defined a psychosocial construct referring to the development among organizational members of shared mental understandings of the organization and its operations [Cousins 2003]. According to Heap [1998] conditions for change and innovation are knowledge, involvement and action. Organizations that find, develop and motivate talented people will gain in the competitive market in which they operate. Various disciplines had used the term and contributed to its evolution [Argyris and Schön 1996; Huber 1991]. Ultimately, Senge [1990] popularized it in his book The Fifth Discipline [Senge 1990], he describes organizational learning as “where people continually expand their capacity to create the results they truly desire, where new and expansive patterns of thinking are nurtured, where collective aspiration is set free, and where people are continually learning to see the whole together” [Senge 1990]. This thesis takes IE as its theorical foundation and focuses on the human relationships and believes that are key factors in its development. Korhonen et al. [Korhonen et al. 2004] connect IE to management and public policy, implying that the industrial systems and network philosophy of IE can be linked with inter-organizational management studies. Other studies research in the field of inter-organizational relationships had dealt on how helping companies at creating value by combining resources, knowledge-sharing, shortening time to market, and gaining access to foreign markets [Barringer and Harrison 2000]. When companies choose to be part of a network where cooperation is needed it is normally due to a variety of interacting causes.

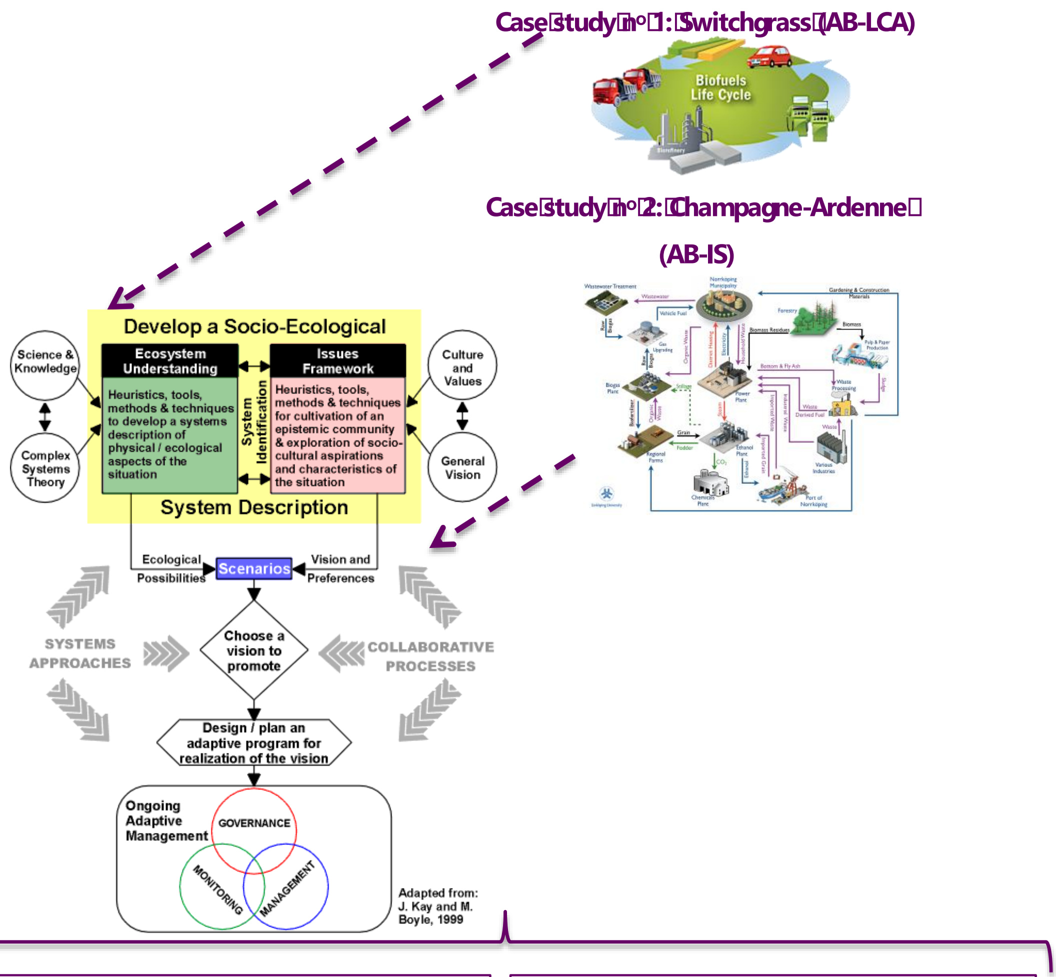
Alter and Hage [1993] states that willingness to co-operate, need for expertise and need for financial resources and shared risk as crucial factors. In the AB-IS case study, cooperation is the central variable influencing IS development; understanding its effect when simultaneously triggered with other variables is relevant.

2.3.2 Systems thinking

The term “system thinking” includes a variety of concepts and fields, such as: mathematics, biology, computer science, physics, biology, etc.… System thinking has its foundation in the field of system dynamics, founded in 1956 by MIT professor Jay Forrester. The methods have been used for over thirty years [Forrester 1961] and are now well established. According to Miller “Systems thinking is a holistic approach to analysis that focuses on the way that a system's constituent parts interrelate and how systems work over time and within the context of larger systems” [Miller et al. 2010]. System thinking philosophy believes that the essential building blocks of a living system are the building blocks of the whole, which none of the parts have. Systems thinking has its ancestors in; complexity theory, open systems theory, organizational cybernetics, interactive planning, soft systems approach, and critical systems thinking [Flood 1999]. Systems thinking seeks to explore things as wholes, through patterns of interrelated actions [Senge 1990; Flood 1999]. System dynamics is a tool to visualize and understand such patterns of dynamic complexity, which will be further discussed in this chapter. A growing literature is focusing on the application of principles from complex systems thinking to environmental issues and IE. Bass [Baas 2005] defines IE is as “a branch of systems science and systems thinking”. He relates system thinking to IE as follows:

- “A system is a set of elements inter-relating in a structured way.
- The elements are perceived as a whole with a purpose.
- The elements interact within defined boundaries.
- A system's behavior cannot be predicted by analysis of its individual elements.
- The properties of a system emerge from the interaction of its elements and are distinct from their properties as separate pieces
- The behavior of the system results from the interaction of the elements and between the system and its environment. (System + Environment of System = A Larger System)
- The definition of the elements and the setting of system boundaries are subjective actions. So the assumptions of the definers or observers of any system must be made explicit.”

A greater appreciation of the integrated, systemic and complex nature of socio-ecological systems has emerged [White et al. 1994; Berkes et al. 1998; Kay et al. 1999; Holling 2001; Gunderson and Holling 2002; Mitchell 2002]. Complexity theory acknowledges the interrelated nature of things as well as emergence, where the whole is experienced as greater than the sum of its part, as well as self-organizing Hierarchical Open (SOHO) system [Flood 1999]. Kay et al. [1999] characterize SOHO systems descriptions as scenarios of how a self-organizing, heuristic, open system might evolve. Such a heuristic framework for an ecosystem approach has been developed by Kay et al., [1999], a modified summary linking this framework to the research undertaken in this thesis can be seen in
Figure 4.



Case study #1

Practical model

Apply the theoretical framework

Identify industrial symbiotic opportunities in agribusiness in the Champagne-Ardenne region, as well as the impact of the behavior of production units on the overall industrial system. ABM modelling is here combined with a GIS and actual data about input and output flows of an industrial ecosystem are used.

Case study #2

Hypothetical model

Test the theoretical framework

Identify the major factors contributing to the adoption of switchgrass by farmers are identified and assessed, and the related effects on the life-cycle environmental impacts (CO2 sequestration and emissions) of switchgrass-derived biofuels are quantified. Focuses on identifying key behavioral triggers for the economic and social development of bioenergy production

Figure 4: An ecosystem approach framework.

(Reproduced from Bunch [2000] and adapted from Kay and Boyle [1999])

Figure 4 highlights that the system behavior is a dynamic non-linear process, therefore the development of alternative scenarios for creating sustainable and effective system is needed through the use of complexity theory modeling tools such as ABM, which be discussed in more details in the following sections.

2.3.3 Assessing sustainability through simulation modeling

2.3.3.1 Why Modeling Systems?

A model is a substitute for a real system [Ford 1999]. They are used to understand and explain the behavior of a complex system over time. Knowing a system's patterns of behavior speaks volumes about its structure. For a decision maker, understanding the structure of a system is a critical first step in designing and implementing effective policy.

According to Borshchev and Filipov [2004] modeling is a "way of solving problems" that occur in the real world. It shows how the system works, by graphing the linkages between each element of the system [Franco et al. 1997]. Modeling is valuable when an overall picture is needed. When problem solver do not know where to start, system modeling can help in locating problem areas or in analyzing the problem by highlighting the different parts of the system and the linkages between them as well as pinpointing other potential problem areas and data collection needs: indicators of inputs, process, and outcomes (direct outputs, effects on clients, and/or impacts). [Franco et al. 1997].

We can distinguish between analytical and simulation models. Analytical models are mathematical models that have a closed form solution; i.e., the solution to the equations used to describe changes in a system can be expressed as a mathematical analytic function. However, analytical solution does not always exist or may be hard to find. Therefore, simulation or dynamic modeling may be used. The process of developing a simulation model involves defining the situation or system to be analyzed, identifying the associated variables, and describing the relationships between them as accurately as possible [Halog and Chan 2006; Halog et al. 2011]. Because of their dynamic nature (energy, material and information flows) traditional analysis tools (mathematical models) fall short because they do not engage with the intrinsic autonomous behavior of network agents [Kempener et al. 2009; Beck 2011; Petrie et al. 2007]. Therefore, the best method to design and analyze industrial ecosystem will be simulation modeling. Our focus in this thesis is to demonstrate modeling method in which this can be accomplished. In the next part, simulation modeling such as System Dynamics (SD) and ABM as well as their potential relevance within industrial network will be discussed in greater detailed.

2.3.4 The System Dynamics (SD) Modeling Approach

Interest in SD is spreading as researcher appreciate "its unique ability to represent the real world by accepting the complexity, nonlinearity, and feedback loop structures that are inherent in social and physical systems" [Forrester 1994]. SD as a method has been in existence since 1961, developed by Jay Forrester [1971] to handle socio-economic problems with a focus on the structure and behavior of systems composed of interacting feedback loops. SD provides a high level view of the system emphasizing the interactions between its constituent parts, as well as the impact of time on its dynamic behavior [Tulinayo et al. 2008]. As a method, it has its focus on the structure and behavior of systems composed of interacting feedback loops. The art of SD modeling lies in representing the feedback loops and other processes of complexities that determine the dynamics of a system [Tulinayo et al. 2008]. "Classical ecological science is about natural eco-systems, and its behavior at a near equilibrium state, that is, at steady-state" [Bohne 2005]. The dynamics emerges from the interaction of two types of feedback loops, positive and negative loops. Positive loops tend to reinforce or amplify whatever is happening in the system. Negative loops counteract and oppose change. These loops all describe processes that tend to be self limiting, processes that create balance and equilibrium. Simulation with SD models is used for learning about the dynamic complexity of systems, identification of optimal policies in existing systems, improvement of system behavior through parameter or structural changes [Tulinayo et al. 2008]. Figure 8 in section 3.3 shows how the different parts of the system are influencing and interacting with each other in a dynamic system

In summary, SD models are feedback-based; "they model systemic problems at an aggregate level over time" [Scholl 2001]. Within an industrial ecosystem, SD can help humans understand the overall behavior of the system over time, including structural changes. Since SD models are feedback loop based, therefore we can witness changes in the system by adding, altering, or removing variables in order to witness the effects that these changes will have on other variables. This procedure can be performed over and over, which will provide us multiple scenarios over time. We will also have access to detailed information about the evolution of each variable, which will give us insights in pinpointing those that require our action and attention. Consequently, this procedure will provide the information needed to choose and implement the most sustainable scenario. Although System Dynamics has not been integrated in the framework methodology of this thesis, it had been considered in the early stages of this research project, more specifically the computational combination of SD and ABM. Appendix F shows this some interesting modeling attempts that could be the starting point of further research project.

2.3.5 The Agent-Based Modeling (ABM) approach

The idea of AB modeling was developed as a relatively simple concept in the late 1940s. Since it requires computation-intensive procedure, it did not become widespread until the 1990s. The aim of ABM is to reveal global consequences of individual or local interactions in a given space [Holland and Miller 1991]. Interacting agents, though driven by a small set of rules, which determine their individual behavior, account for complex and global system behavior whose emergent dynamic properties cannot be explained by analyzing its component parts [Scholl 2001]. In Holland's words, "The interactions between the parts are nonlinear; so the overall behavior *cannot* be obtained by summing the behaviors of the isolated components" [Holland 2000]. Emergence, thus, is understood as the property of complex systems where "much (is) coming from little" [Holland 2000; Holland and Miller 1991].ABMs consist of a space, a design framework, in which interactions take place and a number of agents whose behavior in this space is defined by a basic set of rules and by parameters [Holland and Miller 1991; Miller et al. 2012; Halog and Manik 2011].

The models simulate the simultaneous operations and interactions of multiple agents, in an attempt to re-create and predict the appearance of complex phenomena [Damaceanu 2010]. The process is one of emergence from the lower (micro) level of systems to a higher (macro) level. As such, a key notion is that simple behavioral rules generate complex behavior. This principle, known as K.I.S.S. ("Keep it simple and stupid", an acronym first introduced by Robert Axelrod [Axelrod 1997] is extensively adopted in the modeling community. Another central is that the whole is bigger than the sum of the parts. According to Simonovic, individual agents are seen as rational and considered to act following their own interests, such as reproduction, economic benefit, or social status, using heuristics or simple decision-making rules [Simonovic 2011].

2.3.5.1 Agent-Based Modeling in Industrial Ecosystems

The world is becoming increasingly challenging because our organizations, societies, governments, etc., are becoming more complex. Shrinking resources, growing structural complications such as fragmented markets, deregulation of electric power, natural gas and telecommunication etc., lead to a world which is becoming increasingly complex [Anderson 2012]. To deal with these complexities, ABM has been used since the mid-1990s to solve a variety of organizational and technological problems. Examples of applications include supply chain optimization and logistics, modeling of consumer behavior, social network effects, distributed computing, and human resources management. In these kinds of applications, the system of interest is simulated by capturing the behavior of individual agents and their interactions [Bonabeau 2002]. ABM tools are usually used to test how changes in individual behaviors will affect the system's emerging overall behavior.

ABMs, allow bottom-up simulations of oagents constituted by a large number of interacting parts [Fioretti 2005]. Thus, industrial ecosystems constitute an obvious field of application. The general problem of the behavior of individuals in the face of imperfect incentives lies at the core of industrial ecosystems [Axtell et al. 2002; Andrews 2009]. Therefore, an important role for AB modeling in IE should be to explicitly treat the incentives that face behaviorally realistic agents in empirically credible environments. Here we focus more closely on the methodological aspects of agent models and ways in which industrial ecologists may begin to exploit their capabilities for systems modeling. Agent models have been applied in a variety of contexts of some relevance to IE, including models of resource extraction and trade [Axtell et al. 2002; Batten 2009; Cao et al. 2009; Kraines and Wallace 2006; Epstein

1999] and organizational dynamics [Prietula et al. 1998]. A dissertation uses agents to model ways in which firms adapt to changed regulatory environments [Teitelbaum 1998]. Others models investigate conflicting incentives within firms as barriers to adopting efficient technologies. Agents can also be used to model inter-firm interactions within an industry. The role of the media and other opinion-affecting agents such as citizen groups could be added to such a model, in order to consider the full range of organizational stakeholders that influence private and public decisions.

ABMs are good at revealing emergent macroscopic behavior [Fioretti 2005], they are appropriate when aggregate behavior depends on structures of relations, so it cannot be ascribed to a fictitious "representative agent" [Fioretti 2005; Lane 1993] . Indeed, simple ABMs showed the ability to account for the emergence of social phenomena ranging from wealth distribution to the development of local cultures [Fioretti 2005; Epstein and Axtell 1996]. More flexible than differential equations and yet more accurate than verbal expressions, ABMs "offer to the social sciences a descriptive language that attains sharpness retaining the richness of verbal accounts" [Fioretti 2005; Gilbert and Terna 2000].

From an industrial network perspective, ABM seems to be useful to model large-scale system, by feeding the system with rules corresponding to the assumptions of what is most relevant regarding the situation within the industrial eco-park and then watch the emerging behavior from the agents' interactions. In summary the different tools presented above can be individually used and then integrated to assess the sustainability of an industrial ecosystem. As any organization, an industrial ecosystem has to deal with three dimensions of sustainable development: social, environmental, and economic.

Chapter 3 Background and Framework Methodology

3.1 The agriculture-based product industry as a dynamic industrial ecosystem

A close relationship exists between IE, the goal of greener energy policy and the adaptive management of natural resources such as energy and water. These relationships involve interdependencies and flow dynamics between different types of system (industries, public administrations, environment, etc.) The key role of natural resources use and energy consumption facing climate change threats, suggests that the time is ripe for some of the tools and techniques of complex system science to be focused on eco-industrial research, involving complex material and energy flows across network, distribution, and recycling system. In this thesis we understand the agriculture-based products industry, their associated partners (suppliers, customers, public administration) and the natural environment in which they operate as a complex dynamic system. The implementation of an Industrial ecosystem around this industry is seen here as a promising area of application of sustainable assessment and the development of a low carbon economy. The actors include agricultural cooperatives food processing companies, biomass refinery plant, retailers and institutional agencies.

The use of biomass for the production of fuels, energy and materials is seen by many as an important strategy towards sustainable development. Recent initiatives focus mainly on the production of liquid biofuels and much of the strong support for biofuels is premised on the widespread assumption that they are carbon neutral, promote rural development and may provide an opportunity for countries to decrease dependence on imported oil. Worldwide, efforts to replace fossil energy sources with biofuels are at a critical juncture. Many countries such as the United States, the European Union, China, Brazil and India have enacted national policies promoting the utilization of food and non-food biomass [Bringezu et al. 2009].These include e.g. mandates for blending biofuels into vehicle fuels and national biofuels production targets. Mandates for blending biofuels into conventional vehicle fuels had been enacted in 36 states/provinces and 17 countries by 2006. These mostly mandate blending of 10-15% bioethanol with gasoline or 2-5% blending of biodiesel with conventional diesel fuel [Bringezu et al. 2009].

In the United States, the US Congress passed the *Biomass Research & Development Act of 20003* to promote research and development leading to the production of bio-based industrial products. In 2007 Congress passed the U.S. Energy Independence and Security Act which calls for the use of 36 billion gallons of biofuels nationwide by 2022 comprised of 21 billion gallons of advanced biofuels and the remainder being first-generation biofuels [Earley and McKeown 2009]. The legislation further requires that renewable biofuels must achieve a reduction in life-cycle greenhouse gas emissions. Under current legislation, corn ethanol must achieve at least a 20% reduction in lifecycle emissions, biodiesel and advanced biofuels a 50% reduction, and cellulosic ethanol at least a 60% reduction. In the EU, the *Biofuels* Directive 6 of 2003 introduced the target of a 5.75% market share for biofuels in the transport sector by 2010. Additionally, a communication from COM 20017 outlined that a substitution of 20% of all conventional fossil-based fuels with alternative fuels should be aimed at by the year 2020 [Bringezu et al. 2009]. In 2005, the EU Biomass Action Plan 8 was designed to increase the use of energy from biomass for heating, electricity and transport purposes. The most up-to-date target from 2009 has been defined in the Renewable Energies directive 9 with a *mandatory 10% minimum target* to be achieved by all EU member states *for the share of biofuels* in transport petrol and diesel consumption by 2020 [Nigam and Singh 2011].

Biofuels are divided into first, second, and third generation biofuels depending on the feedstock used for their production. Whereas first generation biofuels are commercially produced using food crops (e.g. seeds, grains, corn, sugar cane, etc.), second generation biofuels utilize non-food sources. These include lignocellulose biomass e.g. originating from waste (agricultural and agricultural residues as well as biodegradable municipal solid waste), corn stover, wood, and miscanthus. Third generation biofuel refers to biofuel derived from algae. According to Dragone et al. [2010] Microalgae are produce 15–300 times more oil for biodiesel production than traditional crops on an area basis, therefore "it is considered to be a viable alternative energy resource that is devoid of the major drawbacks associated with first and second generation biofuels" [Nigam and Singh 2011; Chisti 2007; Li et al. 2008].

Ethanol production for fuel purposes increased from 30 billion to about 67 billion liters between the years 2004 and 2008, whereas biodiesel grew from 2 billion to at least 12 billion liters [Martinot and Sawin 2009]. Recent estimates indicate a continued high growth in worldwide biofuels production [Bringezu et al. 2009]. Despite this growth, liquid biofuels still represent only a small percentage of the world's final energy consumption. First generation biofuels for transport represented only 0.3% of global final energy consumption in 2006, whereas traditional biomass, primarily for cooking and heating, represents 13%. In contrast to biofuels and bioenergy, bio-based materials have so far not received much political attention. In fact, only one political target has been set in the United States to increase the share of biomass-based chemicals from currently about 5% to 25% in 2030. The use of biomass for material purposes is as old as mankind. However, with technological development and industrialization non-renewable materials including metals, minerals and fossil fuels have increasingly started to replace biomaterials in buildings and infrastructures, machineries as well as many consumer goods [Bringezu et al. 2009]. The biomass basis of economies is based to a large extent on agriculture and forestry. Wood is primarily used in construction, production of furniture and paper and cardboard.

Several scientific studies have shown the potential of bio-based fuels, energy, and materials to reduce both non-renewable energy consumption and carbon dioxide emissions in comparison to their fossil- based counterparts [Weiss et al. 2007]. However, agricultural biomass production and processing is also associated with adverse environmental impacts. Agricultural biomass production can have negative environmental effects such as soil erosion, eutrophication of ground and surface waters, and destruction of ecosystems resulting in diminished biodiversity. Cultivation, harvesting and subsequent processing of biomass feedstock consumes fossil energy and requires the energy intensive production and use of artificial fertilizers and hazardous chemicals.
These challenges are just one aspect of the problem. A need to mitigate ecological impacts, particularly greenhouse gas emissions, and energy consumption have

highlighted the need to develop methods capable of addressing economic and ecological uncertainties consistently within an integrated framework. A biobased economy has been recognized as a way to reach a sustainable development [van Dam et al. 2008; Octave and Thomas 2009; Patermann 2012] The concept is a contrast to today's fossil based economy that has emerged during the 20th century and is dependent on fossil fuel. A bio-based economy is one where growth rather is based on renewable biomass from agriculture, forestry, fisheries and aquaculture being used in value-added products in the food, feed, industrial and energy industries [Patermann 2012]. A tool in the transition to a truly bio-based economy is the related concept of biorefinery. In a biorefinery the biomass serves as feedstock for several end products and by doing so reduce waste and contribute to closing loops. From this, it becomes apparent that industrial symbiosis and biorefineries are partly overlapping concepts and that the Agro-industry and its network are an evolving system of complex interactions between nature, physical structure, market rules, and participants (see Figure 5). Participants face risk and volatility as they pursue their goals and make decisions based on limited information and their mental model of how they believe the system operates.

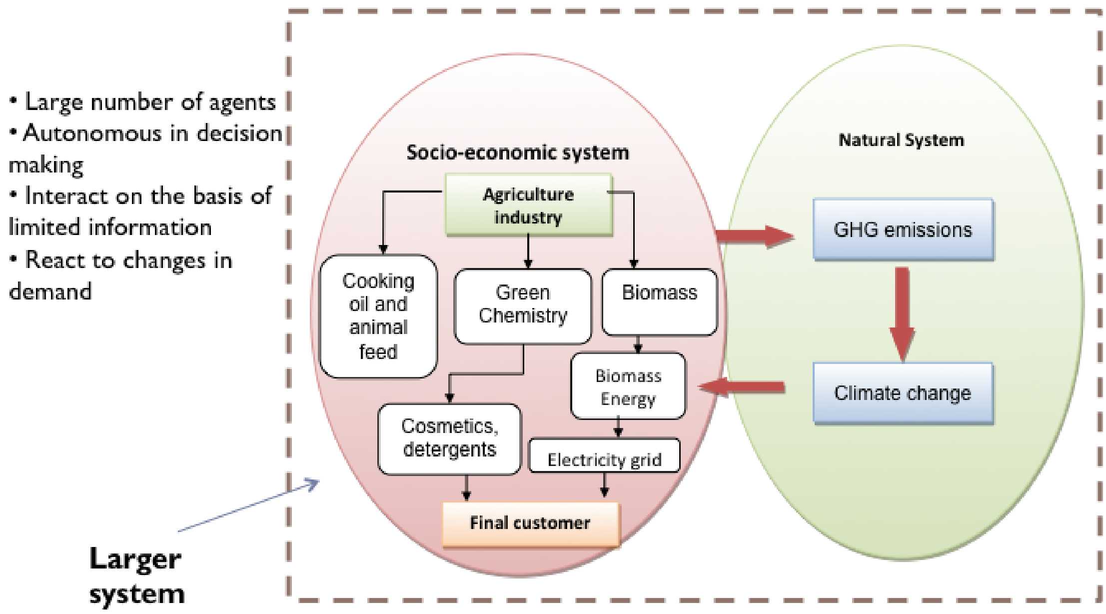


Figure 5: Agriculure-based product industry as a Complex Adaptive System

In practical terms, the first step will be to determine energy and material flows. Then, a network flow strategy is devised and synergies between existing and proposed industries at the site are examined with the assistance of a dynamic modeling software program. Where synergies are identified, those businesses are matched up and the benefits of exchange are discussed. If the flow analysis reveals gaps, then new businesses are recruited to locate at the park. In the meantime, customers for existing energy and material flows are sought. As data are collected from new businesses at the park, a regional database is assembled to further promote exchanges. The final step is to adjust the network flow strategy as companies come and go. At this point, we will have enough information about the ecosystem, therefore resource constraints and hypothesis can be used in a simulation model in order to evaluate different scenarios.

3.2 From Biomass cascading to Biofuel production synergies

Efficient use of biomass with regard to land-use is desirable to reduce GHG emissions, enhance resource conservation, and minimize environmental impacts. Such an efficient use of biomass can be realized by biomass cascading [Arnold et al. 2009] The concept of biomass cascading means to use biomass as feedstock for the production of a material (e.g. construction material, chemicals and bio-based polymers, etc.) first, before it is either recycled and used for further material applications, or the energy content is recovered from the final waste material at end-of-life (Figure 6).

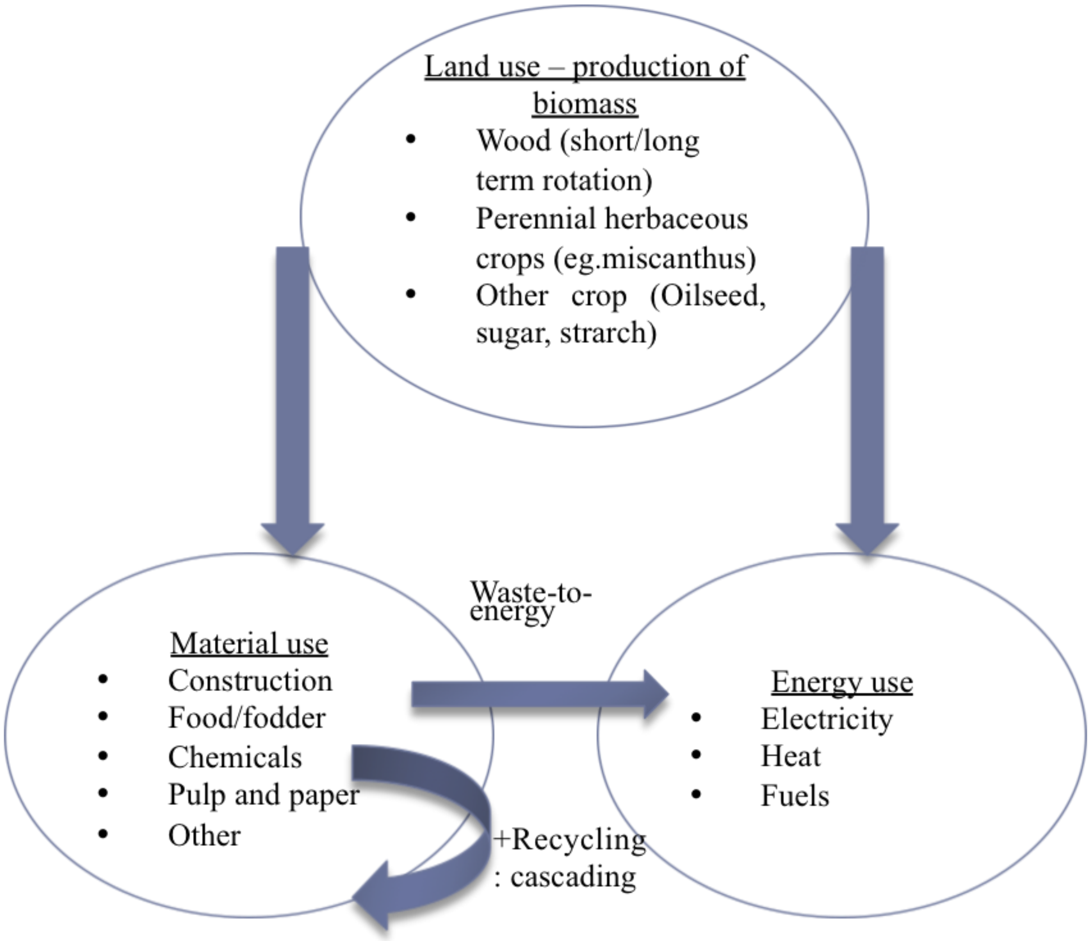


Figure 6: Schematic overview of biomass cascading [Dornburg 2004]

In this way, limited biomass resources and ancillary inputs can be saved and overall resource efficiency increased. The concept of biomass cascading stands in contrast to conventional biofuels production for transport purposes which can be considered as "linear processes" depending on significant amounts of agricultural or forestry production area. The main sectors of bio-materials are pulp and paper, chemicals and construction. In particular the chemical industry is expected to offer new opportunities for biomass utilization with bulk chemicals from biomass having large potentials to substitute fossil feedstock in the chemicals industry [Dornburg 2004] Bio-based plastics and fabrics are likely to become more important in the future [Bringezu et al. 2009]. With regards to construction materials extensive cascading potentials exist, based on the large market share of the sector and a variety of well-established recycling options. A comparative analysis by Weiss et al. [2007] was able to show that the use of biomass for bioenergy and biomaterial production offers significantly higher environmental benefits than direct production of biofuels.

However, competition between the materials and energy sector may act as an obstacle for the prolongation of cascading chains [Bringezu et al. 2009]. In addition, as long as biomaterials are derived from biomass originating from agricultural and forestry activities they will also directly compete with the use of these areas for food production and potentially lead to expansion of global arable land. It is in terms of non-renewable energy consumption, global warming potential (GWP), eutrophication potential, and acidification potential. In summary, cascading use of biomass resources may be a promising concept to decrease land use and GHG emissions for biomass material and energy uses. Material applications that look promising for this concept are bulk chemicals and construction materials.

One way to take the biofuel industry to the next level is to apply the concept of biomass cascading within a symbiotic system by organizing synergies within and outside of the studied production industries. These collaborations can be conducted within the core business of the company, i.e. producing biofuels, or evolve between other processing within the biofuel actors businesses or other industries outside the biofuel industry [Martin et al. 2009].

In this thesis, the adoption of biomass as an energy feedstock and the cascading biomass by-product has been chosen as the core industry for both case studies. In the next section, the framework methodology will be presented followed by a brief introduction to the case studies.

3.3 Methodological framework

This integrated research adopts a systems approach to assess material, waste yields, energy use and consumption, carbon implications, economic advantages, and social impacts of biomass production on spatial and temporal scales. We want to develop dynamic system models that can generate important and useful information, which will help identify unexpected consequences early in the development of alternative material use and energy strategies to avoid costly restructuring in the future. The models would contribute to the charting of sustainable economic policies by enhancing our understanding and knowledge of policies' impacts on a region.

The causal loop diagram below (Figure 7) helps us understand the causal relationships between various factors that influence biomass energy system development. The diagram consists of a set of loops representing the variables connected together. These are: Natural resources, Energy economics, Global economy growth, Socio-economic development, climate change and industrial symbiosis endeavor. These loops are seen as key factors affected by and influencing several variables that control biomass development. Within each loop exist variables and relationships between these variables that are represented by arrows and can be labeled as positive or negative.

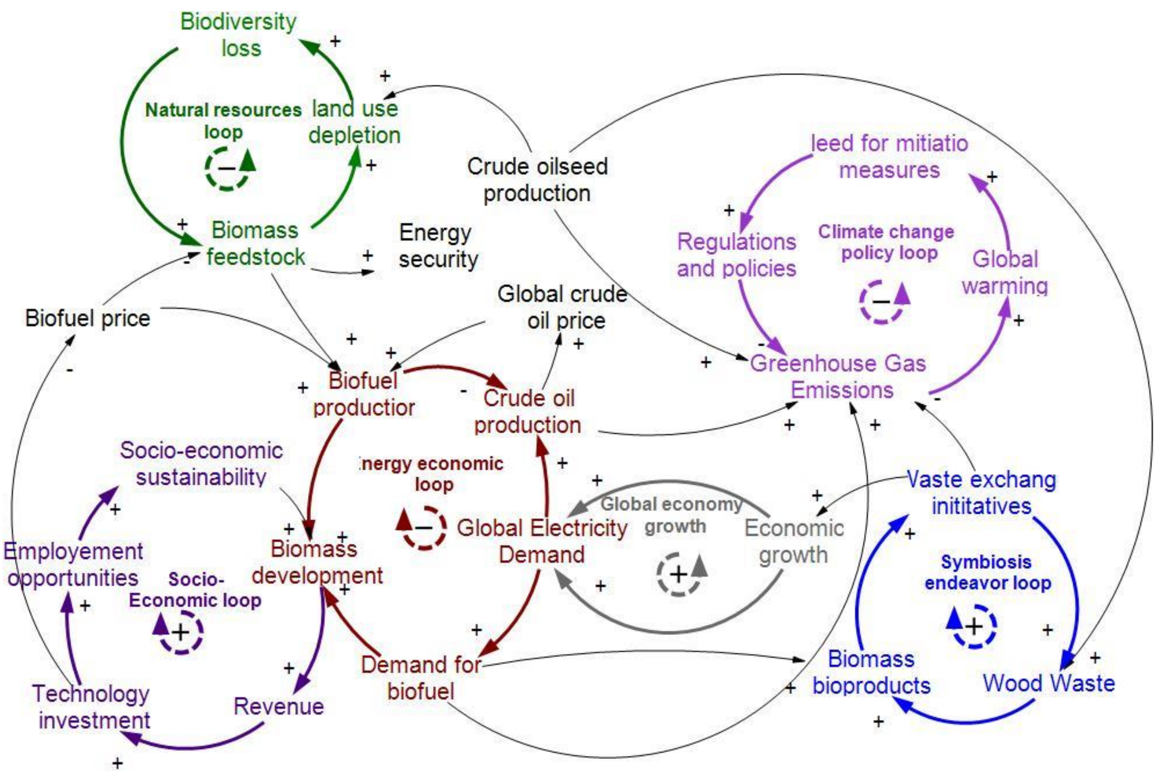


Figure 7: Causal loop diagram of influencing factors in reducing GHG

This causal loop diagram maps out the influences of the various components in the biomass system and how they interact. In addition, the diagram has identified a set of mitigation indicators such as policies and industrial symbiosis alternatives, along with potential impacts and influences:

- **Energy economics** loop considers the profitability of the biofuel production. The higher the biofuel production, the more the biofuel production cost is incurred, which negatively influences the biofuel profitability. Demand and supply of the crude oil determine the crude oil price, which, in effect, influences the biofuel demand by the relationship of substitutes. When the crude oil demand increases, the crude oil price increases, too, but when the crude oil price increases, the crude oil demand decreases. Also, as the crude oil supply increases, the crude oil price decreases, and as the crude oil price increases, the crude oil supply increases. A causal link from the crude oil price to the biofuel demand is positive, meaning that an increase in the crude oil price results in an increase in the biofuel demand. Global energy demand is exacerbating climate change issues and energy prices volatility by reinforcing the demand for energy production.

- **The climate change** loop depicts the influence of crude oil production and policy on global warming: The traditional energy market production cycle is dependent on fossil fuels, here represented by the crude production, increases GHG emissions which contribute to global warming. An increase in crude oil price leads to a higher demand for biofuel, which reinforce biomass production and help reduce GHG emissions that are due to current fossil fuel use. Higher GHG call for the need for more mitigation measures implying the enforcement of regulations and policies in favor of reducing GHG.

- **The natural resources** loop is mainly affected by land use. Biomass expansion can have a negative effect on natural resources because of its consequences on land use and biodiversity. An increase in biomass feedstock influences higher biomass production, which, in turn, necessitates additional land requirements. Higher land use results in more biodiversity loss, which implies depletion in natural resources. On the other hand an increase in biomass feedstock implies more energy security.

- **Global growth economy**, it is a typical self-reinforcing loop, the more global economic growth we observe, the higher the energy demand is.

- **The Socio-economic loop**, shows the impacts of biomass development on social sustainability and technology. Biomass development increases revenue, which provides more allocation of resources for Research and development and technology investment, which has a positive effect on employment opportunities and social welfare. Biomass production encouraged by policies that either enforce carbon charge taxes or subsidize renewable energies can increase revenue for research and development while having a positive effect on employment opportunities.

- **<u>The industrial symbiosis endeavor</u>** loop introduces the alternative of developing waste exchange initiatives implied by the development of biomass and production of the agro-industry. The agriculture production increases the waste production, which can benefit the implementation of waste exchange initiatives and therefore the development of industrial eco-parks. Industrial symbiosis benefits economic growth assuming that the wood waste used in the exchange initiatives allows savings in natural resources purchase.

In summary, the agro-industry system can provides multiple benefits, including energy to local communities, as well as providing synergetic solutions between sustainability and greenhouse gases mitigation. However, large-scale biofuel production raises questions involving land use and productivity (short and long-term), environmental sustainability, social and economic feasibility. Ecological issues mainly encompass the use of fertilizer and pesticide, repercussion on biodiversity, land erosion, hydrology and the type and amount of government subsidies required. This causal loop diagram focus on environmental impacts but other aspects can be added such as jobs loss/or creation etc.; All of these issues can be modeled as variables in a model. Then, change in one or two variables can yield different results in the system behavior, which ultimately will permit comparisons between scenarios.

3.3.1 Models implementation

Industrial ecosystems are the concrete application of closed loop systems, with the resulting symbiosis of organizational decisions continuously changing the character and the configuration of the network [Bichraoui et al. 2013a]. The challenge is to determine the relevant variables to be stimulated within the model to produce scenarios, which will help managers to make decisions that are, at the same time, beneficial for their organization and sustainable for the environment and the local community.

The combined approaches of Life Cycle Assessment (LCA), Geographic Information System (GIS) and Agent-Based Modeling (ABM) help explore various evolutionary pathways of the industrial eco-system under different assumptions about demand in renewable energy, institutional changes, and new technologies. The simulated outcomes will help the further stakeholders to identify future sustainable scenarios, such as maximizing profit while maintaining (or creating) jobs in a carbon-constrained environment. An overview of the model is shown in Figure 8. Both case studies are set on a regional scale and the simulation will take into account infrastructures, land use, and of course actual participants within the industrial system, which is the system boundary.

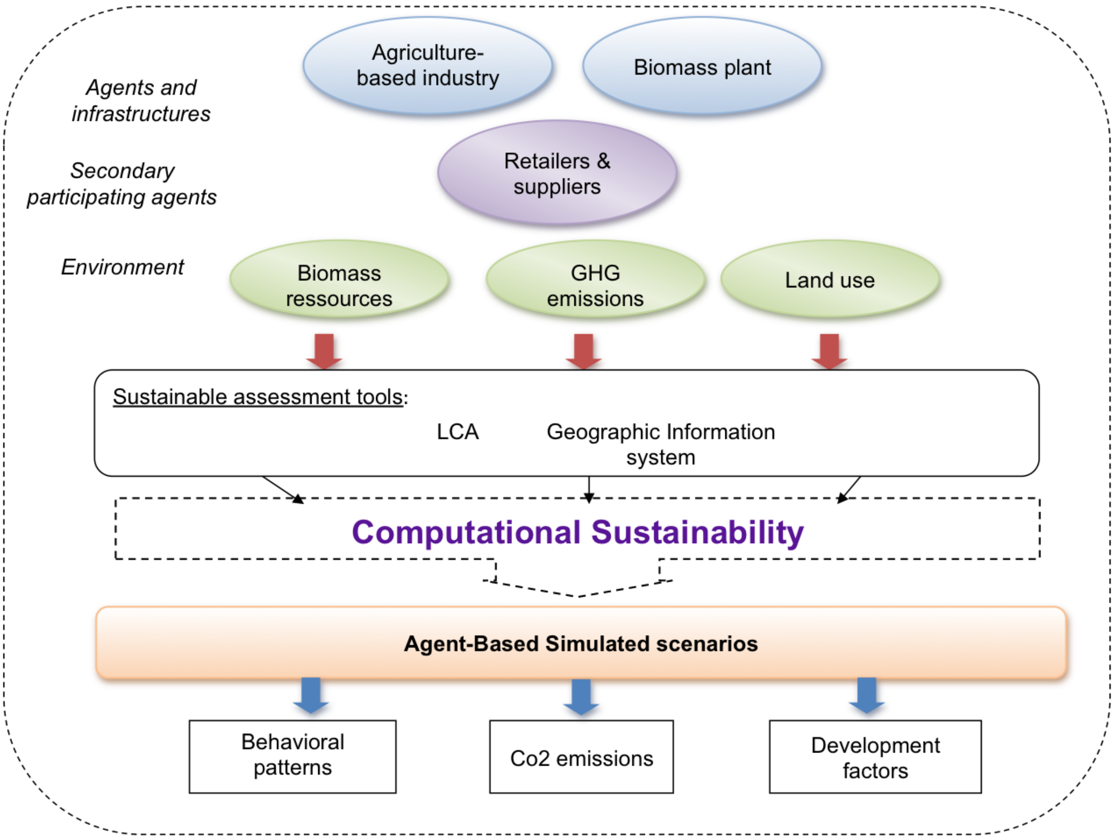


Figure 8: Overview of the combined sustainable assessment and simulation tools to assess the sustainability of the industrial ecosystem

The cases studies are explored through an ABM in order to understand how do the agents behave and what kinds of interrelations and patterns evolve in the system. Translating the model within software enables one to make experiments with the model. The modeling software used in this research is NetLogo. NetLogo is a free open-source modeling environment for developing multi-agent models. It is authored by Uri Wilensky and developed by Northwestern University's Center for Connected Learning (CCL) [Wilensky 1999].

Chapter 4 Case studies and Model construction

4.1 Agent-Based Life Cycle Assessment for Switchgrass-Based Bioenergy Systems

4.1.1 Problem Formulation and Actor Identification

The increasing global demand for energy has motivated a search for alternatives solutions to, if not replace, complement the current fossil fuel based energy production. One of these solutions is renewable energy produced from a variety of biomass feedstock. One of the promising feedstock for bioenergy is switchgrass, a perennial grass native to North America that is a well-adapted to grow in a large portion of the US with low fertilizer applications and high resistance to naturally occurring pests and diseases [Bransby et al. 2005]. Switchgrass-based energy production has a number of potential benefits: reducing erosion due to its extensive root system and canopy cover [Ellis 2006]; protecting soil, water, and air quality; providing fully sustainable production systems; sequestering C; increasing landscape and biological diversity; returning marginal farmland to production; and potentially increasing farm revenues [McLaughlin and Walsh 1998; McLaughlin et al. 2002].

While the properties of switchgrass as a biomass feedstock have been intensively studied, the adoption pathways by farmers for this crop and the environmental impact of these pathways have received much less attention. The Renewable Fuels Standard (RFS2) contained in the Energy Independence and Security Act of 2007 (EISA) mandated that 500 million gallons of cellulosic biofuels be produced in 2012. However, due to several production limitations, the Environmental Protection Agency reduced the amount to 10.45 million gallons based on actual production capabilities (U.S. Environmental Protection Agency, 2012). In addition, the described initiatives by federal and state to reduce dependence on foreign oil and diversify energy portfolios do not indicate that they are optimized for environmental performance. Therefore, data are needed to fill research gaps to determine the aggregate environmental impact of different bioenergy development pathways (e.g., biofuels or biomass electricity); however, since the system is still under development, predictive tools must be used to get relevant information. Such tools for are Life cycle analysis (LCA) and AB modeling. LCA is useful for analyzing well-established supply chains. The use of LCA has significantly influenced policy-making in the energy sector, it provided relevant information on environmental benefits and costs before investments were made in new energy, grid, and storage infrastructure [Hellweg and Canals 2014]. However, LCA faces some methodological challenges, especially for biofuels. Indeed, LCA results can have high uncertainties because the methodology often requires population-based average data are substituted for site-specific data resulting in a potentially inaccurate representation of the study area [Tillman 2000]. LCA also suffers from the use of simulated data and the simplified modeling of complex and adaptive environmental systems such as biofuel supply chains. In their article, Hellweg and Canals 2014 support this notion by stating that "the use of biomass for bioenergy leads to a temporary increase of carbon in the atmosphere, which acts as a greenhouse gas until it is sequestered again" [Hellweg and Canals 2014], which calls for the inclusion of time as a full right element in evaluating environmental impacts.

Consequential LCA (CLCA) is a LCA version that could get us closer to this goal, by "assessing environmental consequences of a change in demand" [Thomassen et al. 2008] and is powerful when highlighting indirect impacts that affects processes [Guinée et al. 2011]. However, it is still of limited use in modeling non linear systems and emerging industries when used alone and the systems that may benefit most from an LCA are emerging, uncertain, and difficult to quantify with traditional LCA methods. AB modeling is proposed to complement LCA by characterizing the dynamic interactions among the system's constitutive components [Davis et al. 2008; Nikolic et al. 2009]. This project has two major goals. First, we will develop an Agent-Based LCA (AB-LCA) framework to help improve the standard LCA modeling technique by overcoming the issues involved with analyzing emerging technologies with dynamic and evolving supply chains. The achievement of this goal will advance the LCA methodology and provide a new tool for environmental sustainability analysis, as well as contributing to filling the gap between LCA and Life Cycle Sustainability Analysis (LCSA). Second, we will apply this improved LCA modeling framework to the U.S. switchgrass bioenergy system (biofuels and biomass electricity) to discover the emerging factor of agricultural producers to grow switchgrass as an energy crop and its environmental impact. The specific research question for this model is: What are the main factors encouraging farmers adoption of a new crop? Sub-question derived from the main question is: ***Can we identify specific social and economic factors that have a specific impact switchgrass LCA?*** Our research establishes an agent-based approach to systems thinking but also recognizes the benefits of life cycle data as an initial parameter for our model. This hybrid approach produces an emergent system that utilizes the strengths of each approach. We then apply our system to model the supply chains of the switchgrass biofuel and bio-electricity industries. The model incorporates the decision-making behavior of farmer agents under different social attributes such as age, education, and familiarity with switchgrass-based ethanol production, risk-aversion toward adoption, as well as selling price structures, and transportation scenarios. We are also able to model the effects that these decisions will have on the sustainable aspect of the system.

Model validation is a critical issue for any modeling approach applied to any system, thus, the model will be tested through a linear regression analysis and comparison to historical data. Sensitivity analysis scenarios to analyze the outcome under little complexity, and to observe if the simulated scenarios converge or diverge. Therefore, the validity of the implementation of the model is critical in assessing the results. The completion of this work will provide a roadmap for the nation and selected states to achieve bioenergy development goals while meeting market demand and minimizing environmental impact.

4.1.1.1 Method and data

The case study that will be used to demonstrate the usefulness of an AB-LCA framework is the switchgrass bioenergy system. Although it has been grown in buffer strips to reduce non-point source emissions from agriculture, switchgrass is not currently cultivated as a commodity crop. In the long run, switchgrass may grow as a dedicated energy crop as envisioned by both existing bioenergy plans (e.g., EISA or state RPS) or proposed pathways such as the "90-Billion Gallon Biofuel Deployment Study" conducted by the Sandia National Laboratories and General Motors [West et al. 2009].

Switchgrass was chosen for this research effort due to a variety of reasons. First, its broad cultivation range allows it to be grown throughout the U.S. In this way, the heterogeneous nature of different policy regimes and logistical supply chains can be explored. Second, like any cellulosic bioenergy option, it can either be combusted directly for heat and/or power or undergo conversion to ethanol. An outline of this process is shown in Figure 9

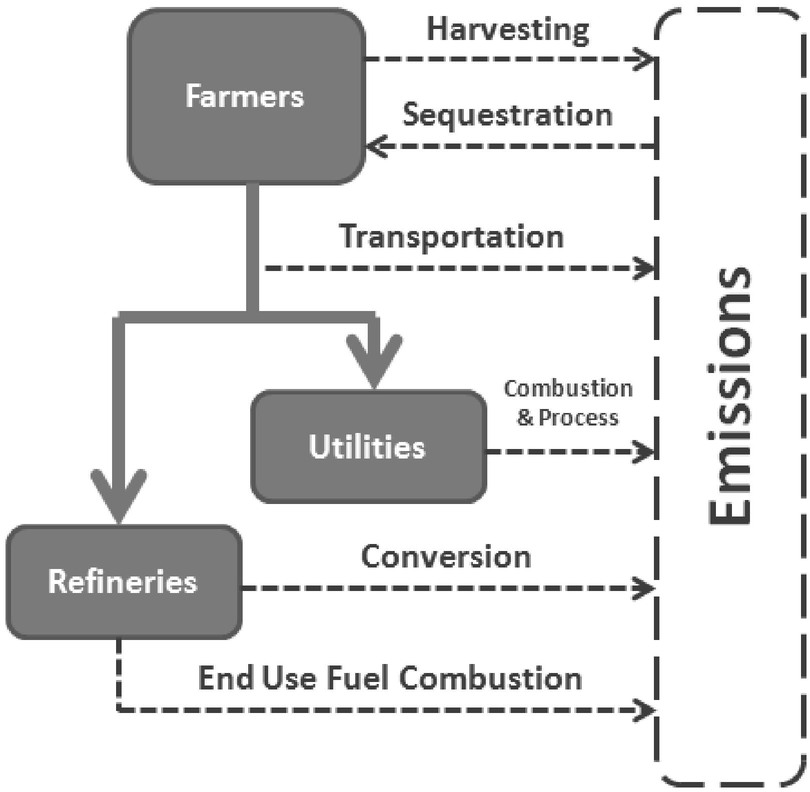


Figure 9: Flow diagram of switchgrass production mass flow and CO_2 emissions

These supply chain options have different environmental profiles. This diversity of supply chain potential creates an ideal scenario to be explored via ABM. Third, the environmental impacts of the switchgrass-to-energy system will greatly depend upon where the switchgrass is grown and the previous land use, which highlights the need for a model. Finally, switchgrass is not currently grown at a large-scale and is therefore an ideal emerging system to model. Corn residues or forestry products generally do not involve a land use change since they exist on parcels of land already producing corn or timber. While these alternate cellulosic feedstocks have their own set of logistical issues to explore, switchgrass is a cellulosic feedstock that may have dramatic growth in the reasonably near term. Unlike corn residue or forestry products, switchgrass represents an entirely new commodity and landowners will only convert to switchgrass if there is good reason to assume a market for this commodity will exist. Given that cellulosic ethanol production is not currently commercially viable, alternate markets such as the heating and electricity industries may be incentivized as an intermediate stage to support a stable switchgrass supply. Due to these complexities, the switchgrass bioenergy supply chain will be highly dynamic and sensitive to policy interventions as it evolves. As such, it is the ideal case study to deploy the proposed AB-LCA framework.

Preliminary research indicates that converting high intensity agriculture such as cotton to switchgrass is expected to reduce nonpoint emissions of fertilizers and pesticides and sequester carbon by increasing the soil organic matter. Growing switchgrass on land previously under contract with the Conservation Reserve Program (CRP) and containing unmanaged grasses or trees has the opposite effect.

As with any modeling effort associated with technology adoption, market forces alone cannot predict user behavior and switchgrass adoption. Landowner decisions to convert to switchgrass will be based on a variety of factors such as economics, risk tolerance, familiarity with the technology, and ease of implementation. Farmer populations tend to be fairly risk averse and slow to change. The fundamental characteristics of landowner behavior and potential adoption of switchgrass have been explored using a Bayesian statistical approach, which is currently under review [Miller et al. 2013]. In this thesis we discuss a particularly interesting application of the model, we aim to study the adoptions factors of new biomass crop by farmers in the state of Michigan. Data such as average age, revenues etc. has been collected on a regional basis through the USDA Quick Stats. Aside from economic factors such as, potential selling price of the biomass feedstock, current revenue and the potential profit generated from planting switchgrass, we looked at dependencies and relationships between personal (endogenous) and economic (exogenous) factors that enter in the decision-making process more specifically how they impact the LCA of switchgrass production.

4.1.1.2 Behavioral pattern of interest

Farmers are assumed to be rational economic actors that are looking to maximize utility. Therefore, only farmers who currently “breakeven” will consider planting switchgrass in order obtain the highest level of utility. Farmers may be extremely risk averse given uncertainty in the market and unfamiliarity with growing a new crop. Thus, understanding farmers’ risk behavior and how it impacts their decisions is important. Farmers’ risk takes many forms relating to production (yield), prices (markets), finance, government policies, and the overall business [Dismukes et al. 2012]. Farmers’ risk perceptions and attitudes towards these different areas affect their decision-making. Among the many factors that may have an effect on adoption, this study will logically hypothesize that farmer’s age, income, familiarity and learning ability will have a significant effect on the adoption of switchgrass.

Initial Hypothesis: The environmental emissions of future biofuel production process can be explained from known system elements (supply of materials or final energy for the production of the energy system). The overall environmental impact of this future bioenergy will be the sum of the emissions taken from these known system elements and estimations of the new process recorded in isolation

Model Hypothesis: Recent Research in LCA and more specifically on dynamic LCA shows that traditional LCA application on future biofuel production system can be greatly distorted because of its static nature and cannot provide confident results on this particular product. Moreover, others factors such as familiarity with the new technology and expected profit are known to be influential in crop adoption and should have some impact on the new crop LCA.

4.1.1.3 Whose problem are we addressing?

Switchgrass may provide farmers with an opportunity to produce a high-value crop on marginal land, or replace land currently used to produce hay or enrolled in the Conservation Reserve Program (CRP). This research will aide in the understanding of how feasible switchgrass production can be depending on farmers demographic and production trends. This knowledge will aide federal, state, and local governments in making more informed decisions concerning laws and regulations pertaining to switchgrass production.

4.1.1.4 Our role

Our role is to develop a model that incorporates important decision-making factors to simulate possible adoption of switchgrass as a feedstock biomass. In order to do this, key factors are defined that affect the decision making process of farmers when considering adopting a new crop.

4.1.2 System identification

4.1.2.1 State variables and scale

The model encompasses the following entities:

1. Agents
    - Farmers: There are the main actors of this model. The strength of this modeling framework is the explicit use of spatially variable data, which cannot be accurately represented with at traditional LCA approach. Here, each farmer possesses various individual characteristics (e.g., age, land size, familiarity, risk aversion, etc.) that will affect their decision-making.
    - Refineries (Fuel Plants): Biofuel refineries process switchgrass into ethanol, which is used as a substitute for gasoline in the transportation sector. Currently, first generation bio-refineries process corn sugars into ethanol. Second generation “advanced cellulosic” refineries have been proven in concept but have not been established on a commercial scale. The switchgrass biofuel supply chain analyzed in our case study uses these second-generation cellulosic refineries. Each refinery agent in the case study has its own operating parameters much like each farmer agent has its own growing conditions. Conversion rates (liters of fuel per tonne of switchgrass), process energy intensity, and location are all factors that vary among refineries. These values need to be set before importing the refineries into the scenario modeler.
    - Co-fired Generation Plants (Electric Plants): Another agent type for the switchgrass case study is co-fired generation plant. These electricity-

generating utility plants can burn dry switchgrass to heat water in a typical Rankine power cycle. Typically biomass is used to supplement a more energy dense fuel such as coal. The percentage of biomass to total fuel mass is called the co-fired percentage. Typical co-fired percentages are around 6%. The scenario modeler will analyze the emissions associated with burning biomass to produce electricity and will compare it to the fuel that it is replacing in the generation plants. Values such as heat rate, parasitic energy loss, and geographic location are set for each generation plant agent before running the scenario modeler.

2. Patches

   They represent the agricultural parcel owned by the farmers. Each patch is a parcel. Farmers can decide to increase or decrease the amount of land they devote to switchgrass at each time step.

A farm agent has its own state, which is updated after every simulation period of one. The state of the farm agent includes personal characteristics and potential gain from planting switchgrass. The important parameters with respect to the individual characteristics of the farmers are detailed below.

Age

We analyze the impact of farmers' age, which is usually found to have a negative effect on perennial energy crop adoption [Rämö et al. 2009; Jensen et al. 2007]. It is in line with the general literature on technology adoption, older farmers being more reluctant to change, or the expected return of the investment being lower. However, Roos et al. [2000] found a positive effect for very young farmers under 35 years old. In Villamil et al. [2008] the effect of age was not significant.

Familiarity

Familiarity is a variable that represents the level of knowledge farmers have about switchgrass. Because switchgrass is a new crop, information regarding its production may not be as widely disseminated as other more conventional crop options. If a producer puts a high level of importance on the discrepancy between his or her familiarity of switchgrass compared to other crops, they may be less likely to be interested in growing switchgrass. Because of this, it is hypothesized that a low familiarity will have a negative effect on interest in growing switchgrass.

Potential income

Income's effect on innovation adoption has been analyzed by multiple studies [eg., Jensen et al. 2007; Norris and Batie 1987; Ellis 2006]. Ellis [2006] found that having a farm income that is lower than 75,000 dollars had a negative effect on adoption. Jensen et al. [2006] hypothesized that greater on farm income would have a positive effect on the adoption of a new crop, but that on farm income per hectare would have a negative effect due to the increased opportunity cost of converting hectares to switchgrass.

Risk aversion

Farmers may be extremely risk averse given uncertainty in the market and unfamiliarity with growing a new crop. Thus, understanding farmers' risk attitudes and how it impacts their decisions is important. Multiple studies on the willingness to take financial risk have analyzed the ways that risk effects adoption of new crops (e.g., [Fernandez-Cornejo and McBride 2002; Fernandez-Cornejo et al. 1994; Daberkow and McBride 1998]). These studies have found that early adopters tend to be less risk averse than late adopters or those that never adopt the innovation. Daberkow and McBride [1998] describe late and non-adopters as those who perceive a large amount of production and financial risk associated with a new crop adoption.

Economic performance

Generally, farmers with larger financial capacities are considered to be more prone to technology adoption, particularly if the adoption requires some important investment, like in switchgrass. Breen et al. [2009] did not find any significant effect of either the farm income or the solvency of the farm business on farmers' interest in energy producing crops. Moreover, Jensen et al. [2007] tested a land-productivity variable (net farm income per hectare) and found that it impacted negatively farmers' willingness to grow switchgrass. However, Jensen et al. [2007] was not able either to show any significant effect of farmers' indebtedness on the willingness to grow switchgrass.

4.1.3 Concept Formalization

4.1.3.1 Design concept

For this model to useful in the future, its building aims to be modular, meaning that the designs any of which components can be replaced without breaking the overall functionality. For example, some the agent personal attributes and global parameters of the farmers (Table 1) can re-used in further models.

Overview

The scale of our AB modeling framework focuses on the farmer's decision-making in adopting a new crop and its impact on its LCA. Farmers are assumed to be rational economic actors that are looking to maximize utility. Therefore, only farmers who currently breakeven will consider planting switchgrass in order to obtain the highest level of utility. Breakeven farmers are farmers who are experiencing a profit, even minimal, but not a loss with their current crop. Farmers can be unwilling to adopt a new crop because of the uncertainty of the market and lack of experience in growing this particular crop. Thus, understanding farmers' risk behavior and how it impacts their decisions is important. It is of particular interest to incorporate these factors and to look at their effect on the environment especially when a traditional LCA does not allow it. This study hypothesizes that farmer's age; income, familiarity and learning ability will have a significant effect on the adoption of switchgrass and that these effects will have an indirect impact on its LCA.

Emergence

The emergent effects we are looking for in this model are the environmental consequences of the decision making process the farmers make when a new crop is being introduced. The AB-LCA of the farmers consists of fifty hypothetical heterogeneous farmers. At the beginning of each growing season, depending on their financial situation and personal characteristics, the farmers choose to plant or not switchgrass. It is assumed that young age and high familiarity increases naturally with the number of farmers adopting switchgrass. Emergence will occur from the collusion of individual characteristic over time and global variables such as the selling price of switchgrass.

Adaptation/Learning

In this model, farmers adjust through social learning by first re-planting only if they made a profit the previous year, and by remembering the surface area planted and increasing this area if profitable. Adaptation is also triggered by the "learning" procedure; farmers have the possibility of "looking" around them and imitating the most frequent behavior. The decision of a farmer depends on his level of risk aversion, as well as his forecasts of future economic conditions, which update with time as he makes new observations of prices, costs, yields. The farmer also updates his characteristic (age, income etc.) at each time step. Table 1 below shows the model parameters.

4.1.3.2 Model Parameters

Table 1: Switchgrass AB-LCA Model Agent attribute parameters

Personal Attributes	Domain/Description	Unit
Age	Randomly distributed around Average-age =47. *(M=35, SD= 15)*	Year
Education	Randomly distributed around Average-education = 1. *(M=1, SD= 3)*	Year
Risk aversion	(*Ra* < 1.0) Randomly distributed. *(M=0.5,SD=0.1)*	Index
Familiarity	(*Fa* > 1.0) Randomly distributed. *(M=4, SD=2)*	Index
On the fence?	True/False. Farmers who currently breakeven but their other personal attribute level do not qualify them to adopt	Boolean
Mind changed?	True/False. Farmers who were “on the fence” but “Learned” from their neighbors and decided to imitate their behavior by adopting.	Boolean
Profitable?	True/False. Is Revenues form *switchgrass – Expenses > 0?*	Boolean
Agricultural Attributes		
Nb of field owned	Nb of field owned 10 acres (1 patch = 10 acres)	Patches
Acres owned	Nb of field owned 10	Acres
Plant SG?	True/False	Boolean
Nb of field planted	Nb of field planted 10	Patches
My area planted	Nb of field planted 10	Acres
Initial percent of planting	Random-float 0.4	Percentage
SG Harvested	SG harvesting Area SG yield	Acres
Memory planted	[list]. Remember the amount of acres planted	Number
Average distance to refinery	Randomly distributed. *(M=60, SD=30)*	km
Economic Attributes		
Total fixed cost	Fixed cost per acre acres owned	$
Total variable cost	Variable cost per acre acres owned	$
Total cost	Total fixed cost + Total variable cost	$
Current revenues	Base yield acres owned price of base	$
Current profit	Current revenues – Total cost	$
Potential revenues	SG yield acres owned price of SG	$
Potential profit	Potential revenues – Total cost	$
Breakeven?	True/False	Boolean
Switchgrass Revenues	SG harvested price of SG	$
SG profit	SG revenues - (Total cost per acre My area planted)	$

Global variables are parameters that affect the interactions of agent-sets in the model and are not specific to any agent. In our case study, global variables are parameters that are categorized into the three pillars of sustainability, in order to report on economic, environmental, and social impacts of the system. Before running the model, these parameters must be set by using the sliders on the Graphical User Interface (GUI). Their values affect the scenario outcomes, thus a new scenario is created for each iterative change of any of these variables. Table 2 summarizes these sustainable variables.

Table 2: Switchgrass AB-LCA global sustainability variables

	Domain/Description	**Unit**
Economic		
Price of switchgrass	[200,600]	$/tonne
Price of base crop	[200,600]. Price of crops currently planted that could be replaced by switchgrass	$/tonne
Environmental		
CO_2 (growth)	Total CO_2 emissions accumulated during the growth phase	Tonnes
CO_2 (ethanol generation)	Total CO_2 emissions accumulated during the ethanol production phase	Tonnes
CO_2 (electric generation)	Total CO_2 emissions accumulated during the electricity production phase	Tonnes
CO_2 (ethanol distribution)	Total CO_2 emissions accumulated during the ethanol distribution phase	Tonnes
Social		
Learning ability	True or false. If it is true, farmers who expect increased profits from adopting switchgrass but decided not to adopt will be able to change their perspectives on market uncertainty and risk aversion by "learning" from their neighbors.	Boolean

4.1.3.3 Model narrative

Each model time step (tick) represents a growing season session. The time frame for this model is 50 ticks. The diagram below summarize the model process regarding the decision making process of each agent (Figure 10).

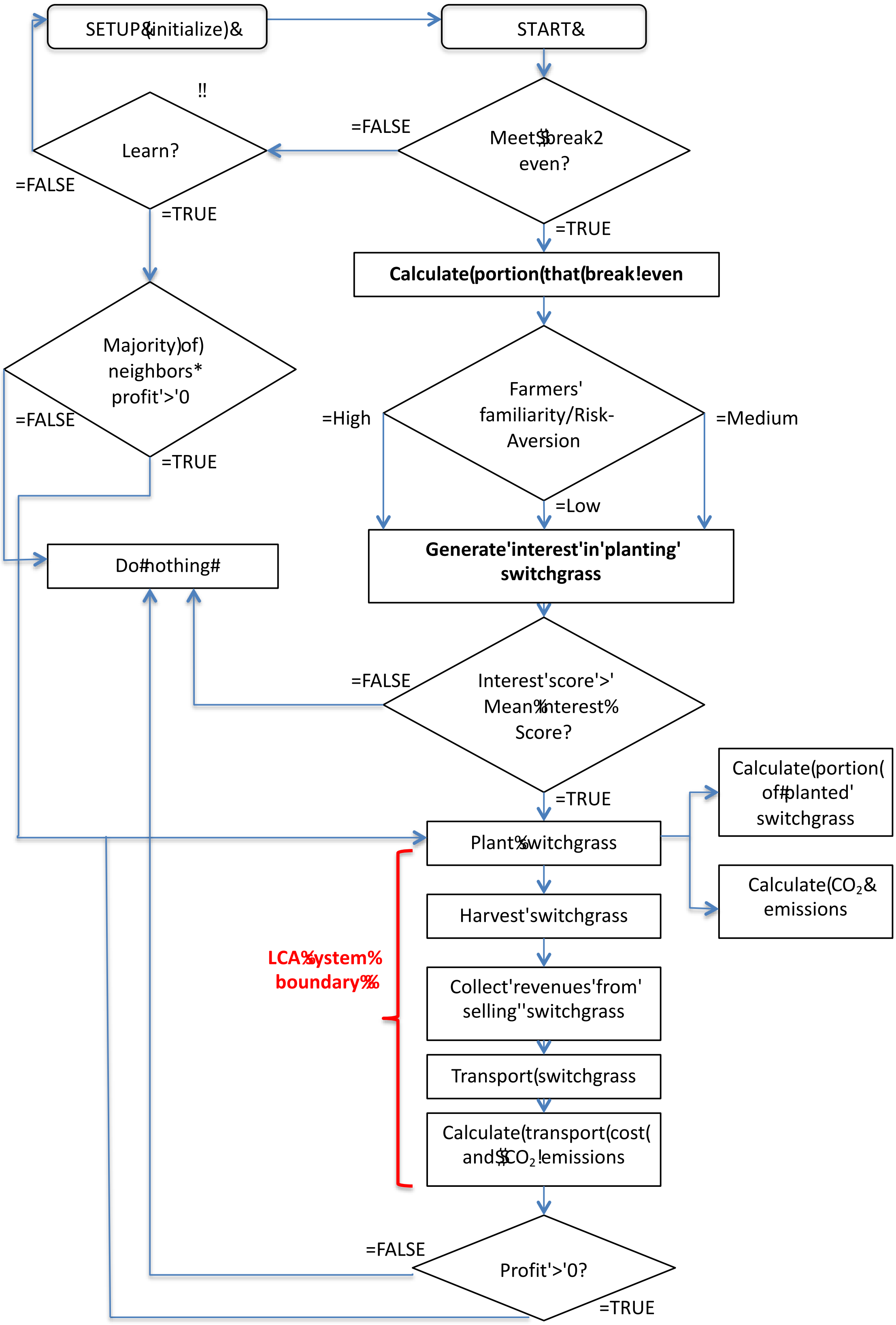


Figure 10: AB-LCA Model Flow diagram

4.1.3.4 Process overview and scheduling

Farmer agents decide at the beginning of each growing season whether to continue their previous year's cropland allocation. The growing season is simulated and switchgrass carbon sequestration is calculated. At the end of the growing season, the model calculates farmer's revenues and determines their profitability, and accounts for the tailpipe emissions when the fuel is eventually used. To better understand the model conceptualization, we present below the detailed model scheduling which is a description of the agent routine and their actions for every iterations, At every time step, each agent performs the following tasks in a chronological order:

1. At the beginning of each simulation year, each farmer compares their current revenues to the expected revenues from planting switchgrass. The farmer proceeds to the next step only if the potential profit is higher than the current profit.
2. Each farmer has distinct individual attributes including age, familiarity with switchgrass, level of risk-aversion, and level of education (see Table 1). Farmers determined their eligibility to plant by comparing their level of familiarity, risk-aversion and education to the overall average in the system. Farmers with attribute over the average level will adopt switchgrass in their land. They Farmers will plant switchgrass on a portion of their land, which is randomly determined based on a normal distribution.
3. At the end of each simulation year, the amount of harvested switchgrass for each farmer is calculated by multiplying the yield with a post-harvesting loss rate. The yield is randomly determined through a normal distribution (yield source: McLaughlin and Kszos 2005). The post-harvesting loss rate is randomly determined with a normal distribution [Samson 2007], representing production losses during harvesting activities such as storage, processing and transportation.
4. Farmers decide to sell their switchgrass to either a biorefinery to produce bioethanol or a power plant to generate electricity. All farmers with switchgrass feedstock send all of it to the refinery. The

decision-making of this part of the model is not studied, therefore no competition between refinery is in place in the current model, they just sell all of their feedstock to the closest refinery, see pseudo code below:

IF

age of farmer < average age and

Familiarity with switchgrass > average familiarity with switchgrass

and

Risk aversion < average Risk aversion and

Education > average education

THEN

[Plant switchgrass]

Return qualified farmers

5. CO_2 emissions from each process of the life cycle of the system are calculated using life cycle inventory (LCI) data (Appendix E) from GREET model [Argonne National Laboratory 2012]. The LCI includes CO_2 emissions sequestrated by switchgrass plantation, emissions generated from harvesting, transportation fuel use in logistics, power generation, and biofuel production, and emissions avoided by replacing fossil fuels or fossil fuel-based electricity.
6. Only profitable farmers that grow switchgrass in the previous simulation year will replant in the next year.
7. Farmers who did expect more profits but not plant in this round of simulation have an opportunity to "change their minds" by learning from their neighbor farmers with a certain radius. If the majority of their neighbors plant switchgrass and are profitable, they will plant switchgrass in the next simulation round.

4.1.4 Results

4.1.4.1 Model verification

The aim of verification is to ensure that the model works as intended [Dam et al. 2012]. Because of the mix of non-linearity and uncertainty regarding parameter value distributions and variation, a sensitivity analysis is required to verify AB models [Burgers et al. 2010]. The model is verified through sensitivity analysis to determine if the model output significantly changes when the value of an input variable is changed. The results of the sensitivity analysis will help verify the model robustness by checking if the effects of parameter variations are coherent or can be explained by the model hypothesis. We divided the simulation results into two different variable observation categories: endogenous variables and exogenous variables. Endogenous variables are related to personal attributes (described in Table 1) while exogenous variables are the potential profit farmers expect to make from selling switchgrass and the cost of production (variable plus fixed cost). Overall, we simulated 120 scenarios of our system with 10 repetitions each, which equal to 1200 simulation runs and analyzed the variation of the main parameters of the model. The data retrieved from the combination of parameters detailed above were analyzed using R [R Core Team 2013], an open-source programming language and software environment for statistical computing and graphics, to explore the data-set which was generated by tens of thousands of model runs.

The simulation results on the average number of farmers adopting switchgrass with different levels of familiarity to switchgrass, risk aversion, and education (Figure 11) show expected patterns. For example, only farmers with the high and medium levels of familiarity with switchgrass are likely to adopt. Farmers with the low level of familiarity are not likely to adopt. On the other hand, it is expected that the high level of risk aversion hinder farmers' willingness to adopt. However, the results show the opposite. It can be explained by the fact that the most influential factor for adopting a new crop is the expectation of making a profit. The potential of making more profit and being somewhat familiar with switchgrass seem to be enough for farmers to make the adoption decision. We also find that the level of education does have a significant impact on farmers' adoption decisions. In particular, farmers with high and medium levels of education tend to adopt right away, while farmers with lower level of education do not.

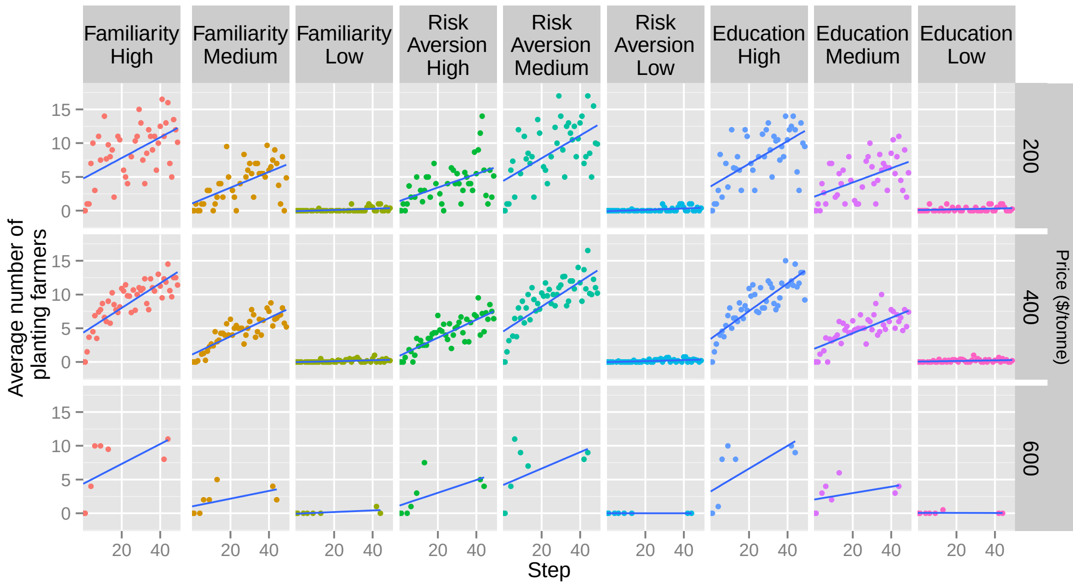


Figure 11: Influence of Endogenous factors: Risk Aversion, Familiarity and Education paired with price of switchgrass on switchgrass adoption

As mentioned in #7 of the farmer's scheduling, farmers who did expect more profits but not plant in the previous round of simulation have an opportunity to "change their minds" by learning from neighbor farmers with a certain radius. The concerned farmers, called "on-the-fence", survey their neighbors up a certain radius (radius of influence). If the majority of its neighbors planted switchgrass and made profits, "on-the-fence" farmers will imitate their neighbors by planting switchgrass. Experiment results showed in figure 12 aim to check for the combined effects of learning ability and radius of influence by neighbor farmers. On the lower part of the plot, we can clearly see that a significant amount (approximately 40%) of farmers adopting switchgrass are those who were "on-the-fence" and eventually changed their minds by learning from neighbors.

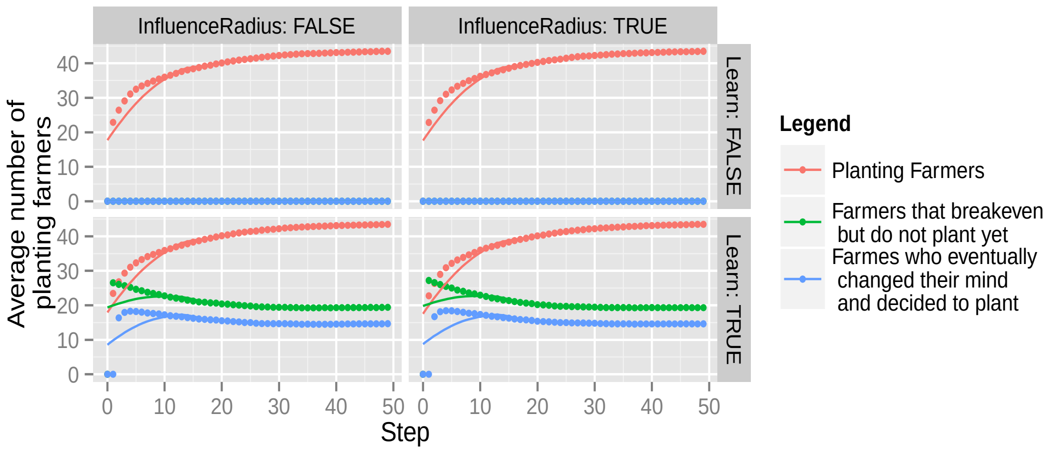


Figure 12: Influence of the learning algorithm and radius of influence on switchgrass adoption

Figure 13 shows that expected profits significantly impact the adoption of switchgrass by farmers. Interestingly we find that farmers that experience high and medium costs of production are also the ones who tend to adopt switchgrass, whereas farmers who have low costs of production tend not to. This can be explained by the fact that cost is part and is proportional of the overall expected revenue, meaning that a high cost means a high-expected profit. Therefore the cost variable is not a determinant factor in farmers' decision-making.

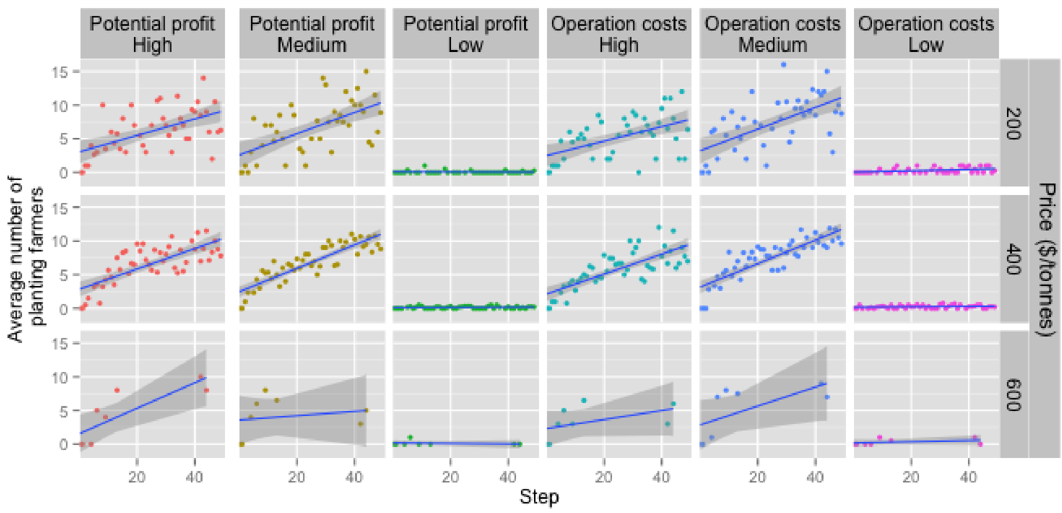


Figure 13: Influence of Exogenous factors: Potential profit expected from selling switchgrass and farm operation costs paired with switchgrass price on adoption

Figure 14 shows the comparison of CO_2 emissions of switchgrass-based bioenergy with fossil fuel-based energy that is replaced by the switchgrass-based bioenergy. We observe that CO_2 emissions from the switchgrass-based bioenergy are lower than those for fossil fuel-based alternatives with limited variations. For switchgrass-based bioenergy, its life cycle in our study includes crop growth, harvesting, transport, ethanol and electricity production, and the use of ethanol as transportation fuels. Note that emissions from land use change are not considered. Depending on the type of land converted to switchgrass plantation, the amount of CO_2 emissions sequestered can be significantly different. Including impacts of land use change is a direction for future model improvement. We compare switchgrass-based bioenergy with its fossil fuel counterparts on a functionally equivalent basis. Note that this doesn't calculate the difference in impact associated with switching from conventional fuels to switchgrass. This just compares the CO_2 associated with equal amounts of energy produced from different fuel sources. For example: if the model showed that 1000 liters of fuel were produced and 500 MWh of electricity were produced from switchgrass, this script will calculate the CO_2 impact from producing conventional fuel (gasoline) with equivalent energy content to that in 1000 liters of switchgrass fuel, and also the CO_2 associated with producing 500 MWh of electricity from conventional sources (coal, ng, etc.). To figure out the CO_2 impact from utilizing switchgrass, the user will need to define a total market demand for fuel and electricity.

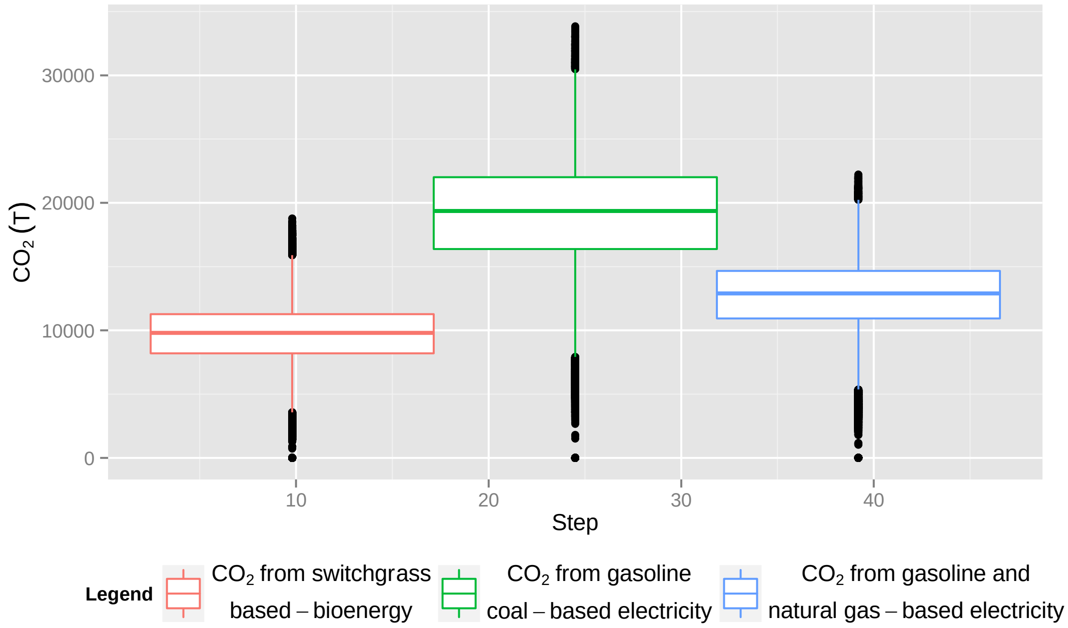


Figure 14: CO_2 emissions from the switchgrass-based bioenergy system comparing with using fossil fuels to produce 500 MWh electricity and 10,000 liters of transportation fuel.

In order to identify specific social and economic factors that have particular impacts on the LCA results, we examine the correlation of each factor with the different stages of LCA as shown in Figure 15 and 16. The plots in the lower left panel of Figure 15 are the paired plots of individual attribute variables for farmers (age, familiarity with switchgrass, risk aversion, and education) and LCA results by different stages of switchgrass-based ethanol (switchgrass growth, ethanol generation, electricity generation, and ethanol distribution). Values of the column variables are used as *X* coordinates, values of the row variables represent the *Y* coordinates, and the diagonal histograms reflect the marginal distributions of the variables. In the upper right panel, correlation coefficients are reported scaling the font size to reflect the absolute value of the coefficients. Figure 16 shows the similar results for exogenous variables including the price of the base crop, price of switchgrass, production cost, and potential profit. In Figure 16 we notice that plots pairing the different stages of LCA as a function of age (purple boxes) are the only plots that display a non-linear relationship. During the growth phase, the U-shaped curve accounts for the sequestration of CO_2. Since the vast majority of farmers are grouped around the average age, the amount of CO_2 sequestered is at its highest (bottom of the curve). When the "pool" of famers is either too young or too old, we observe an expected pattern of less carbon sequestration. The other plots show consistent results but with inverted U-shape curves. All other individual attributes show linear positive relationships, however weak. This indicates that individual attributes of farmers have limited impacts on switchgrass-based ethanol LCA results, although they are inherent to each farmer and enter at the very beginning of the decision-making process.

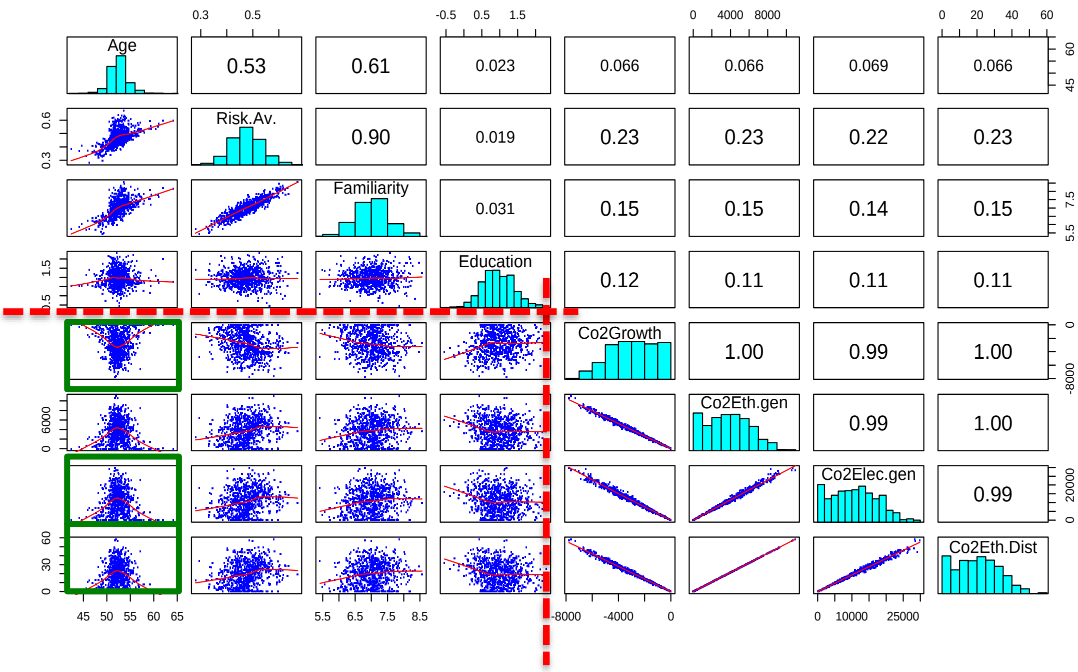


Figure 15: Scatter plot correlation matrix of endogenous attributes effect on LCA.

The plots in the lower left panel are the paired plots of personal attributes variable and different stages of switchgrass-based ethanol are displayed. Each plot examines the linearity and impact of transformations for the personal attributes (age, Familiarity, risk aversion and education) and the variables for each LCA stage (growth, Ethanol generation, electricity generation and Ethanol distribution). Values of the column variable are used as X coordinates, values of the row variable represent the Y coordinates and histograms on the diagonal reflect the marginal distributions of the variables. In the upper right panel, correlation coefficients are reported scaling the font size to reflect the absolute value of the correlation.

In figure 16 we find that selling prices either for the base crop or switchgrass has no direct impacts on the LCA results. However, “potential profit” (pink boxes) as a function of switchgrass selling price and switchgrass production shows strong correlations with LCA results at different stages. The higher level of profit is expected by the farmer, the more they adopt and more CO_2 is either sequestered or emitted during the life cycle stages. The potential profit that famers expect to make seems to have a major impact on LCA results.

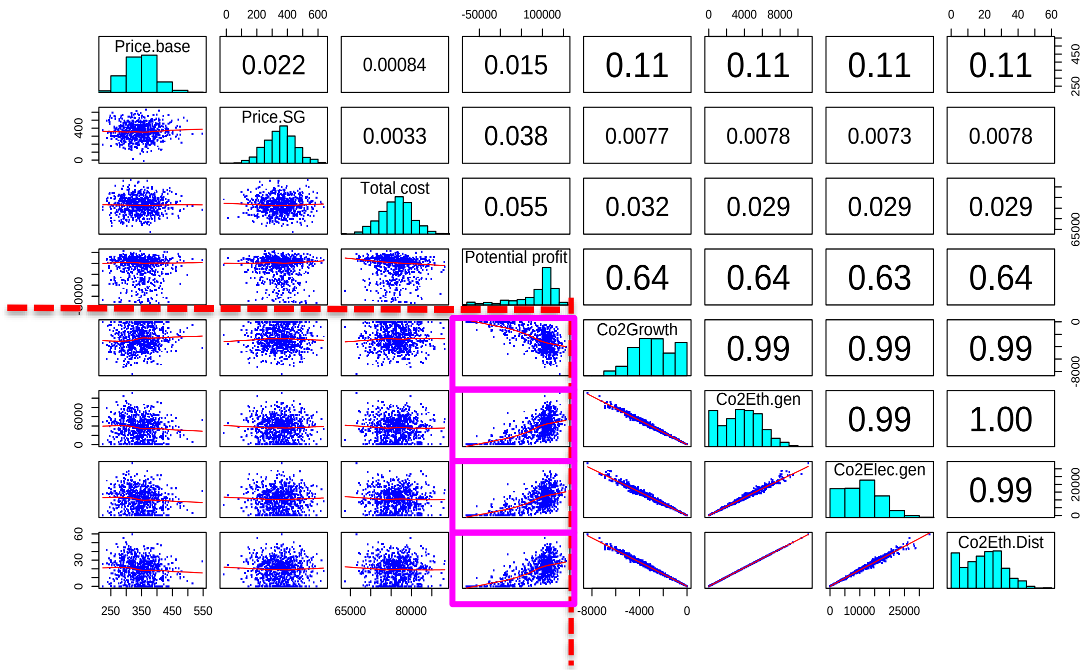


Figure 16: Scatter plot correlation matrix of exogenous variables effecting the LCA results.

4.1.4.2 Model validation

The model is validated to ensure the model simulation reflects the real-world system it intends to describe. Chappin [Chappin 2012] identifies two methods for model validation in genera: static and dynamic. The static method aims at comparing sampled experiments where samples are collected from distinct groups without respect to time. The dynamic method, on the other hand, is a temporal experiment where samples are usually collected over time in order to uncover progressive system behavior. The former does not apply to time-dependent data, while the latter does. In this study, we use both methods by 1) Comparing the simulation results with observed data, and 2) Testing the model's fitness through a multiple linear regression analysis. Just like switchgrass, genetically engineered soybeans (GE soybeans) were new crops being introduced to the market and involved the same actors (farmers). We choose to use historical adoption data of GE soybeans in the U.S for model validation. The rationale is that, if our model can reproduce the adoption pathways of new crops similar to switchgrass, it can generate meaningful predictive results for switchgrass adoption.

Validation by comparing to observed data

Figure 17 shows similar trends of new crop adoption from our model simulation and the historical adoption of genetically engineered (GE) soybeans. We observe rapid adoption when new crops being first introduced. The adoption rate slows down and later an equilibrium is then reached. Indeed, U.S. farmers have widely and consistently adopted GE crops since their introduction in 1990s, despite uncertainties regarding consumer acceptance and economic and environmental impacts [Fernandez-Cornejo and Hendricks 2003].

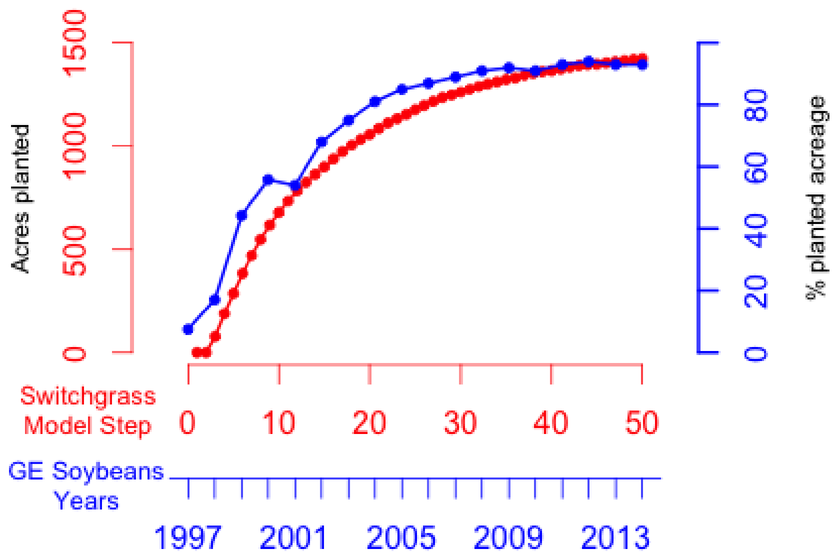


Figure 17: Model simulation results comparing with historical GE soybean adoption.

Validation by testing the model's fitness through a multiple linear regression analysis

A multiple linear regression model is applied to explore the relationship between independent variables and a dependent variable by fitting a linear equation to simulated data [Happe 2005]. By evaluating the significance of individual independent variables to the dependent variable, the multiple linear regress analysis can help validate assumptions made in the model. Note that given the intrinsic complex dynamics in ABM where the result of an output variable change as the simulation runs, this method on its own is not sufficient to claim any proof of validity. Instead, it is considered to be one of the techniques for ABM validation.

For this study, we choose the number of farmers planting switchgrass and the area of land for GE soybean plantation as the dependent variables. Independent variables include farmers' age, education level, learning ability, familiarity with new crops, risk aversion, selling price of the new crop, and revenues. The results (Figure 18) show the predictive power of each independent variable. The thick line represents the 1st standard deviation range. Variables that are away from the "intercept line" and with longer ranges, such as the selling price of switchgrass, revenue, and selling price of GE soybeans, are statistically significant. If they are left of the intercept line, those variables have positive effects on adopting the new crop. To the contrary, if placed on the right of the intercept line, variables have negative effects on new crop adoption. In our switchgrass ABM, the selling price of switchgrass seems to have a negative effect on adoption, but its effects can vary with a great level of uncertainty. On the other hand, variables on education level, learning ability, and familiarity with new crops show to have positive effects on adoption, but are less significant than variables on price and revenue. This multiple linear regression analysis confirms that the independent variables chosen for our ABM have statistically significant impacts on the adoption of new crops, using either artificially simulated results for switchgrass or historical data on GE soybeans.

Figure 18: Coefficient plots of multiple linear regression analysis.

4.1.4.3 Summary of the results

The primary purpose of this study was to determine what identify the main factors encouraging farmers adoption of a new crop and more specifically identifying and understand how the social and economic factors that have a specific impact on switchgrass LCA. An ABM was built in order to identify these variables as well as the main emergent pattern that stems from multi-agent interaction. Overall, the general design of the model in predicting planting trend seems to fit the real system as it showed similar pattern with GE soybean adoption evolution. The calibration results showed that the AB-LCA model was able to reproduce expected patterns as far as the main variables affecting the decision making for adoption. Indeed, it did confirm the assumption from the literature that factors such as age, education and selling price are influential factors, however, they also showed that the extent of each variable is not necessarily what we would expect, for example age and education do have an effect but it seems that their significance is limited, its effect might have been hinder by the other internal variables, therefore a model specifically focusing on this issue would help confirm or infirm this assumption. On the other hand, price and expected profit have a significant effect on the decision making process. Indeed the model results shows that expectation of any profit even low will have a positive effect on adoption but seem to have a direct impact the LCA. The findings of this research have indicated which farmers with high and medium level of familiarity even with a high level of risk-aversion are among the most likely adopt a new crop and that expected revenues are the most significant factor in this process. Switchgrass market still being inexistent, expected revenues should be of are of particular importance to policymakers in helping them develop policies to facilitate the development of this market. Further version of the model should consider extending the LCA analysis to more impact categories, as well as adding more sophisticated economic mechanisms such as change in demand of transport fuel supply. ABMing has been shown to add fineness to life cycle analysis with a theoretical case study. The calculations from this theoretical case may not correlate perfectly with real-world case studies each location will have its own spatially explicit parameters. However, the methodology employed in this case study remains valid. Further work will apply this methodology to a “real world” study area with actual farming practices, land covers, and relevant policy scenarios.

4.2 AB-IS Model for the development Industrial Symbiosis

4.2.1 Problem Formulation and Actor Identification

What makes an Industrial Symbiosis (IS) initiative successful? Industrial ecologists have addressed this question by identifying several pathway for IS emergence including self- organizing [Chertow 2007; Ehrenfeld and Gertler 1997] organizations facilitating [Paquin and Howard-Grenville 2012; Hewes and Lyons 2008] and top-down planning [Gibbs and Deutz 2007; Chertow 2007]. Brand and Bruijn [1999] suggests five categories of barriers that need be overcome when establishing an industrial ecology approach in a region or park. The suggested categories of barriers are: technical barriers, behavioral barriers, economic barriers, political barriers, and organizational barriers. However, very little has been done on identifying and understanding the actual individual and collective factors in participant’s decision-making process that are determinant for IS development as well as its consequences on the industrial system over time. The focus of this case study would be to check our assumption that emergent behavioral pattern can be drawn to help promote IS initiatives. Rather than system prediction, this model means to lead to a better understanding on how to unveil symbiotic opportunities within an industrial ecosystem.

The main goal of this AB-IS model is to determine how actors, represented by the plant manger, within an industrial ecosystem can make decisions that are not only are in their own economic interests, but also stimulate the global benefits of the entire industrial network. Behavioral issues, because they involve human decision making, are much more difficult to identify with precision in order to assess and solve; therefore, an important role of ABM in IE should be to explicitly treat the behavioral characteristics that favor the emergence of sustanaible activities within an industrial ecosystem [Bichraoui et al. 2013a]. **The main research question of this model is**: What level of endogenous and exogenous factors (cultural cooperation, social learning ability etc.) is necessary for IS development and durability? **Sub-questions derived from the main question are**: Can we identify a balance between the exogenous factors (observed cooperation culture in the region etc.) and the endogenous factors (learning, level of trust and doubt) that would be optimal for IS development? Can these findings be replicated to other regions?

4.2.1.1 Method

This model is applied to a case study exploring at the development of regional Industrial symbiosis around the agricultural-based product industry in the Champagne-Ardenne region (France) where a circular supply chain initiative, limited to the flow circulation of cereals and beats waste and by-products, is already in place (see Figure 19). Champagne-Ardenne is a European crossroad lying on the main roads from Paris to Germany and from the UK or Belgium to the south of France, where over 60 percent of its land is dedicated to agriculture (crops, livestock farming and vineyards). Here, we envision that this local circular supply chain initiative can be extended to become an IS endeavor that goes beyond the agriculture industry by involving other local industries with symbiotic potential. Therefore, closing, as much as possible, the material cycles and implementing energy cascading by optimizing local resource use and exchange implies new type interactions between actors, each with its own motivations, which may have conflicting interests. Thus, AB modeling will be used to model their decision-making process and study these interactions that will reveal the system emergent pattern.

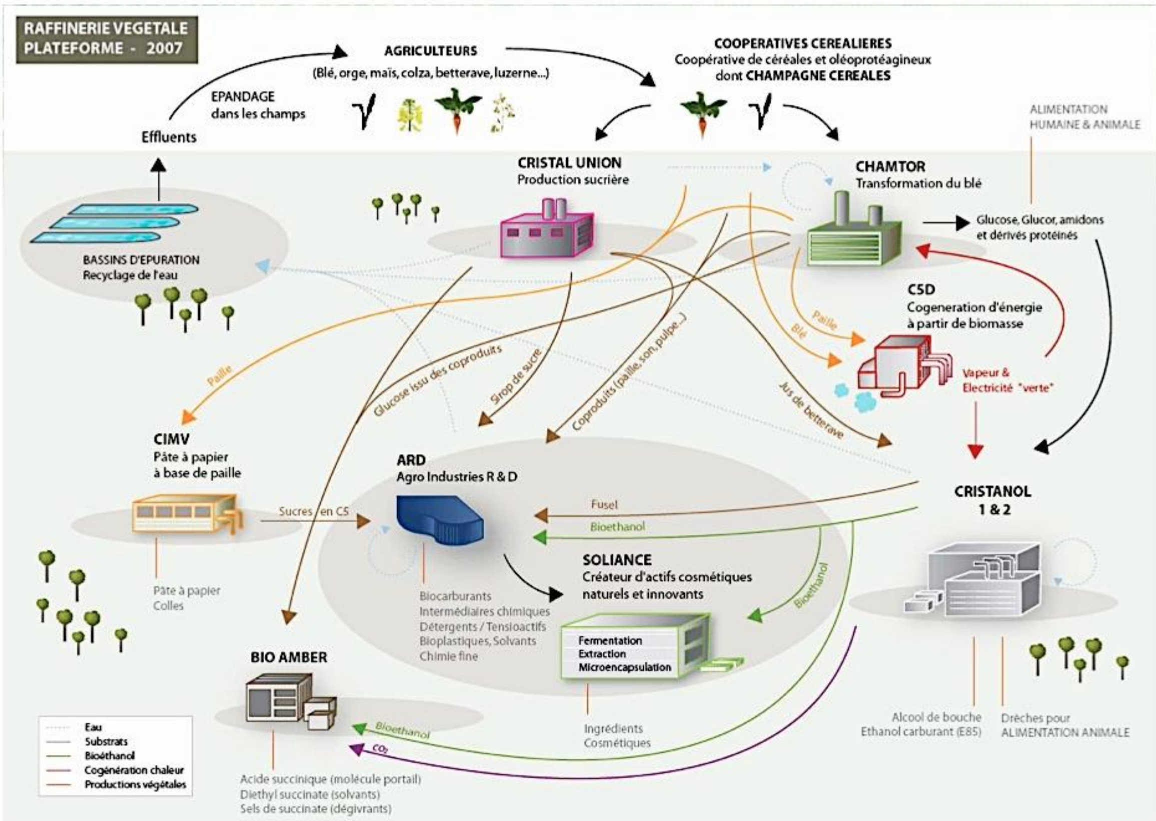


Figure 19: Current industrial symbiosis initiative in Champagne-Ardenne [Rous 2012]

4.2.1.2 Behavioral pattern of interest

IS networks emergence is of two main conditions: Self-organization and pre-planning. In this project, either condition could be the starting point of for this model. Indeed, both emergence type conditions face the same issue: How do we get the main actors (plants) to start exchanging materials and energy?

The behavioral pattern of IS is a function of manager's trust and involvement ability and the result of their reaction to change in the environment. According to Sterr and Ott [Sterr and Ott 2004], "stable eco-industrial regions…develop through a solid foundation of comprehensive information transparency…In order to realize suitable output-input connections, mutual trust among the industrial actors and the willingness to cooperate are essential" [Sterr and Ott 2004] Secretive or non-cooperative corporate cultures that hinge on individual behavior can greatly affect the emergence of a network

Initial Hypothesis: There is no standard framework for IS emergence and development. Each case is rigidly context-dependent, therefore it is very difficult to draw general success factors that could help identifying "ideal" context for IS implementation.

Model Hypothesis: Industrial networks are the result of individual components that forms a system. Each component (plants, supplier etc.) possesses general behavior characteristic (cooperation level, social learning etc.) And follow the same general business behavior constrains by economic expectations. Therefore, modeling these aspects could reveal a behavioral pattern on which actions can be implemented to help IS development.

4.2.1.3 Whose problem are we addressing?

We are addressing the policy makers and industrial manager's problem on possible industrial symbiosis implementation. Policy makers would have an interest on knowing what type of policy is the most appropriate, Industrial managers as being the main actor, can visualize, through geographic layer display, the material and energy symbiotic flows network.

4.2.1.4 Our Role

Our role is to use our knowledge of system (region culture, social and economic fabric of the region) to develop a tool that would help policy makers and industrial managers on possible industrial symbiosis implementation. The focus would be to check our assumption that emergent behavioral pattern can be drawn to help promote IS initiatives. Rather than system prediction, this model can ultimately lead to a better understanding on how to unveil symbiotic opportunities within an industrial ecosystem.

4.2.2 System identification

4.2.2.1 Entities, State variables and scales

The model encompasses the following entities:

1. Agents: They are the plants, represented by plant managers. In this model, 47 plants had been selected, 11 of them being already involved in a local symbiosis endeavor, the main activities are: sugar refinery, cereals and oil-seed grains agricultural cooperative, pulp and paper mills, plastics factories, cement plants, and biochemical transformation plants (Figure 19 and Figure 20)
2. Patches: They are the cells where the plants are located, each plant releases CO_2 on the patch underneath it.
3. Links between agents that represent the exchange of materials: if materials (inputs and outputs) are available. Links will be created between the plants. This model uses actual quantitative input data to represent the symbiosis development, Table 4 summarizes the input and output flows for each participating plant.
4. GIS layers: Currently used as the geographic display of the roads, and the location of the plant. The plants use truck to exchange material with each other, in this model CO_2 emissions from transportation is calculated using the distance between travelled during the delivery stage.

Figure 20 below summarize the different steps to gather necessary data for this model

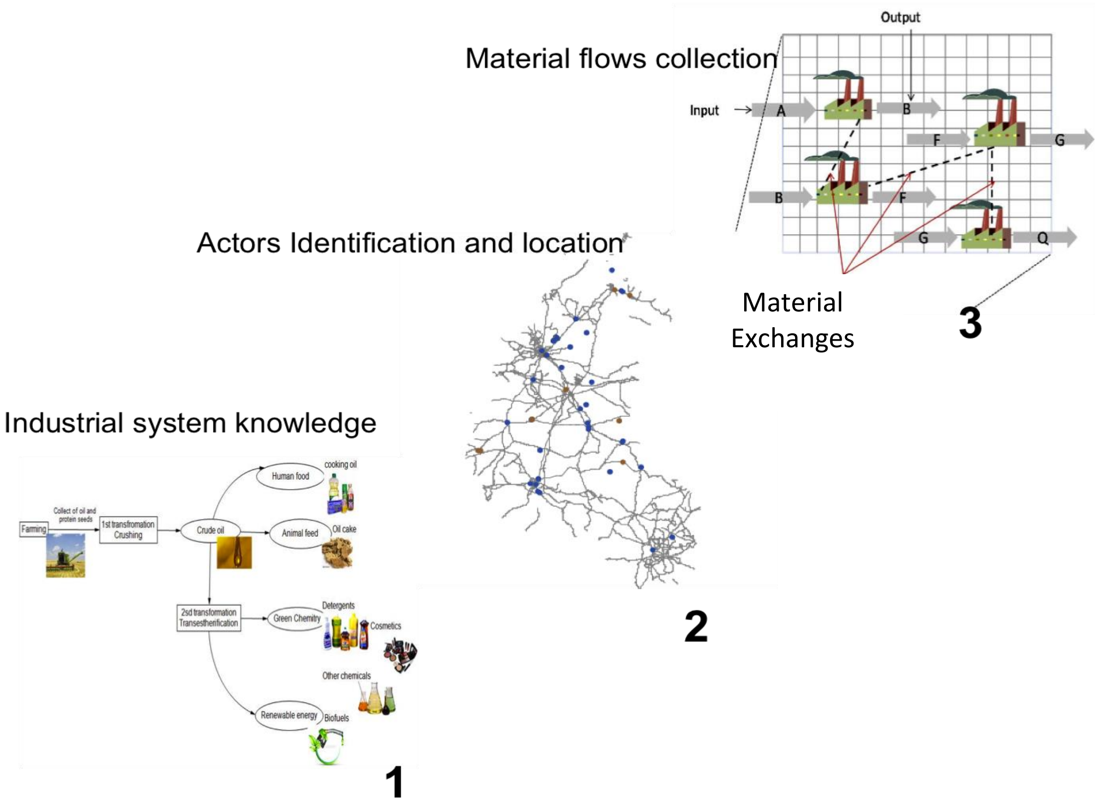


Figure 20: Regional symbiosis AB-IS Framework

4.2.2.2 Data collection

Data was collected mainly to parameterize model simulation. They have been collected from Life Cycle Inventory, websites, public and internal documents to validate simulation model at micro-level. GIS datasets representing the motorways, trunks, primary and secondary roads, rails, rivers and canals were imported and converted to Netlogo coordinates system, Table 3 presents the datasets and the data sources used in this study and Table 4 shows a sample a the compiled data inventory for this model. Finally, Table 5 shows the parameters used in this model.

Table 3: AB-IS datasets sources

Name/type	Format	Data source
Roads (primary and secondary, motorways and truncks)	Shape	OpenStreetMap data www.openstreetmap.org and http://download.geofabrik.de
Participating plants	Shape	Google Earth https://www.google.com/earth/
Land cover (Parcels)	Shape/	Registre parcellaire graphique (RPG) 2010

	Raster	http://www.geoportail.gouv.fr/donnee/48/registre-parcellaire-graphique-rpg-2010
Water treatment facilities (not used in this version of the model)	Shape	Portail d'information sur l'assainissement communal http://www.assainissement.developpement-durable.gouv.fr/

Table 4: AB-IS input data (extract): List of participating plants

	MMT CO_2	Inputs				Outputs				Location	
		In.1	Qty	In.2	Qty	Out.1	Qty	Out.2	Qty	Lat.	Long.
Soufflet Ag.	100	Fertilizers	12800	Wheat seeds	40000	Wheat	60000	Straw	10000	48.857	4.483
Luzeal	100	Lucerne	10000	Beets	5000	Animal feed	20000	Granule	4000	49.412	4.487
ARD	106	Beet Pulp	10000	Glucose	5000	Bioethanol	5000	Detergents	10000	49.336	4.146
Ciment Calcia	83	Limestone	10000	Shale	20000	Cement	80000	Lime	10000	48.758	4.571
Peugeot Cit.	115	Iron	300000	Carbon	50000	Cast iron	390000	Steel blast	10000	49.737	4.750
Efigrain	100	Wheat grains	40000	Biofertilizer	1500	Wheat	30000	Corn	10000	48.717	3.737
Resinoplast	44	Crude oil	1000	Salt	1000	Vinyl	33000	Vinyl scraps	2000	49.258	4.031
Dislaub	106	Beet Pulp	10000	Biochem.	2000	Purif. solvants	10000	Purif. Alcohol	5000	48.226	4.132
C5D	80	Straw	15000	Wheat	5000	Steam	2500	Electricity	2500	49.336	4.146

4.2.3 Concept Formalization

4.2.3.1 Design concept

Overview

The scale of this AB-IS focuses on plant manager's decision-making in getting involved in a symbiotic flow exchange initiatives within a regional network. Plants managers are rationale agent and base their decision first on material need. They use a certain amount of each input each week for their production process, if one or more of this input is available in the right quantity in the network, they will then initiate a partnership with plant that has the material. Their decision is also influenced by exogenous factors such as the global level cooperation of the system, and endogenous factors such as their learning ability. In order to keep the building and analyze of the model manageable, we have made several simplifications and assumptions to formulate the behavior rule. This study does not incorporate prices and market fluctuation and during the exchanges session, the flow is then the maximum amount with which the supplier can meet the need from the re-user.

The emergent effect we are looking for in this model is the ability of the plant managers to develop exchanges of materials following the cultural cooperation spread over the network, according to their individual involvement (doubt and trust index), by imitating the behavior of their neighbors. At this stage of the model, the number of links created and the total number of plants that become partnered measures the IS performance. It is assumed that cooperation increases naturally with the number of exchanges. Emergence will occur from the collusion of cooperation over time and individual involvement.

Collectives

At the beginning of the simulation plants managers are grouped into two subpopulations (breed groups) according to their own involvement ability algorithm: <u>The pioneers and the followers</u>. The pioneers are the ones who have a higher involvement index, above the involvement index threshold. The followers are the ones below the threshold. When the simulation starts, only the pioneers start exchanging. Then, if the number of 10 exchanges is reached within the network the followers imitate the pioneers' behavior by looking for partner to start exchanging. Over the course of the simulation, the plants are divided into two groups differentiated by their behavior: Partnered and Non-partnered (regardless of their breed). Partnered plants are the ones who successfully found one or more exchanges and create " links" between each other. Non-partnered plants are the ones that do not succeed in developing exchanges within the network.

Adaptation/Learning

ABMs are able to simulate learning at both individual and population levels. The literature identifies three ways on how learning can be modeled; "As individual learning when agents learn from their past experience; As evolutionary learning, when the population learn because some agents ''die'' and are replaced by new and more fit agents, improving the population average; And as social learning, in which some agents imitate or are taught by other agents, leading to the sharing of experience gathered individually but distributed over the whole population" [Gilbert 2004]. In this model, the plants adjust through social and evolutionary learning by finding and choosing new input materials from their neighbors that correspond to their own needs. They will only pick input materials that are suitable for their production processes; they are also limited in the number of exchanges made in order to be more realistic. Adaptation is also triggered by the learning and memory algorithm. Unsuccessful plants that do not make exchanges because of their lack of cooperation can "look" at their neighbors and imitate the most frequent behavior within a certain radius; therefore, an initial low level of cooperation can be compensated by " social learning" within the industrial network. They also learn by "memorizing" other past partnership of other plants (see trust transitivity in the next paragraph). Their memories, is an adaptive trait since their learning can alter their behavior.

Interactions

Plants interact directly by searching for input materials among fellow plants, they can also check other plants memory, if they have a partner in common, they will preferably partner with this one. If they succeed in doing so, a link is created between the plants. They also indirectly interact by having the possibility of imitating each other's behavior. In the "real world", interactions within industrial ecosystem may exist between two plants with no relationship between with one another. Under these conditions, we can find the trustworthiness of a plant based on the testimony of past experiences given by other intermediate plants: That is what is called “the trust transitivity problem” [Qiu et al. 2010] In social networks, participants’ trust is one of the most important factors for their decision-making. This necessitates the evaluation of the trustworthiness between two unknown participants along the social trust paths between them based on the trust transitivity properties (i.e., “if A trusts B and B trusts C, then A can trust C to some extent”) [Liu et al. 2011]. The path with trust information linking the source participants and the target one is called a social trust path [Hang et al. 2009].

Stochasticity

Stochasticity is used within the cooperation probability as well as for the trust and doubt index which uses random numbers to create a stochastic approximation of the number of cooperators, pioneers and followers to reward the symbiosis. If there are exchanges during a time period of 10 ticks in a row, then create a new participant.

Observation

Observation is graphically displayed on the interface. The first observation is the total number of exchanges made over the industrial network, since it is the goal of a successful symbiosis. The other major observation is the number of “partnered-plants” under different conditions (high or low cooperation level, learning procedure being “TRUE” or “FALSE”). Another observation is the amount of CO_2 emissions created over the course of the simulation, and the amount of CO_2 saved.

4.2.3.2 Model Parameters

Table 5: Symbiosis AB-IS model parameters

Parameters	Domain	Description
Endegenous attributes		
Material and energy inputs/ outputs	List	Each plant has a set of inputs and outputs, a production capacity (T/year), Million Metric ton of CO_2, which is the average CO_2 for the industry
Location	GPS coordinate converted to Netlogo coordinate	GPS location
Behavior type	Index. Randomly distributed. *(M=35, SD= 15)*	Positive behavior is defined as having found materials to exchange and therefore getting "partnered" with another plant. The behavior of this partnered plant will be marked as behavior = 1. Otherwise, the non-partnered plant will be marked as behavior = 0
Trust index	Index. Randomly distributed. *(M=35, SD= 15)*	Each agent has a trust index randomly distributed between 1 and 5. 1 being a lowest level of trust and 5 the highest level of trust a plant can have. Trust will increase the likelihood of getting involved in the symbiosis and getting partnered.
Doubt index	Index. Randomly distributed. *(M=35,* SD=15)	To balance the trust index, each agent has a doubt index, also randomly distributed between 0.5 and 0.9. The doubt index is mean to inhibit the trust of plant managers
Partnering memory	List	Each plant remembers past partnership, through the "link memory" algorithm of each plant, which lists the plants found at the other end of undirected links connected to the plant
Learning ability	Boolean True/False	This is one of the fundamental aspects of the model. Social learning is an important feature in decision-making. In this model, each plant has the possibility of "learning" from its neighbors and adapting its behavior accordingly. Each plant has the possibility to imitate the most frequent behavior (behavior 1 or 0) within a radius determined by the user, between 1 and 5 patches around the four cardinal point of where the agent in position (North, south, west, and east).
Exogenous Attributes		
Cultural cooperation probability	[0,1]	Frequency of cooperators determined by the "Cultural cooperation probability" slider controlled by the user. The higher % of cooperation the higher is likelihood to get partnered.

4.2.3.3 Model narrative

Each model time step (tick) represents an exchange session. The time frame for this model is 500 steps. Because the plants input data (production capacity, MMt CO_2 etc.) are in ton per year, the assumptions for the flow exchanges are the following:

- One exchange session per day
- All quantitative data (annual production capacity, annual amount of Input 1, Input 2…Output 1, Output 2… MMt of CO_2) are spread out over the year and therefore divided by 300 days.
- Mere identical flows are matched and consistent coding has been used for input and output flows.
- Preliminary process that might be needed in some situation to alter the flow has not been taken into account in this version of the model.

Figure 21 below describes the main process regarding the decision making process of each agent.

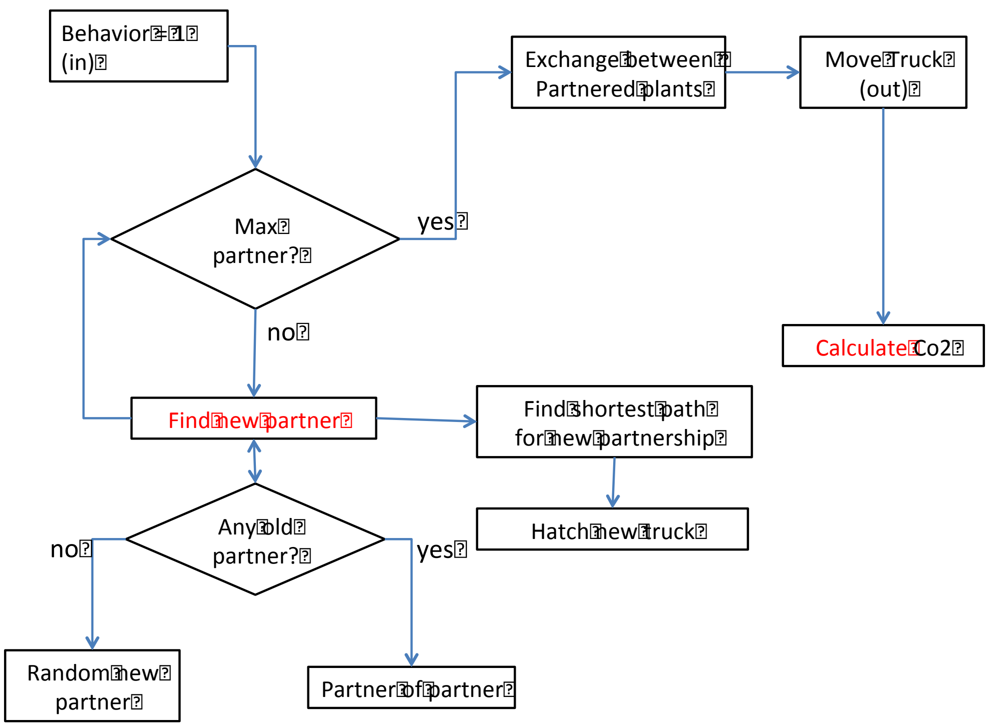


Figure 21: Regional symbiosis model simplified flowchart

Before, getting into the model in more details, I would like to state some important assumptions regarding the nature of the by-product exchanges:

1) While raw material variability is not considered, a stock system has been design (see Figure 22) which deduct each amount of by-product exchange from a total list. 2) All exchanges are assumed to be rush orders,

3) No transport constraints are present. If enough inventories are present at source, replenishment orders are satisfied immediately by sending materials,

4) No materials are stored in the plant and there is no delay in transit from the factory to the store.

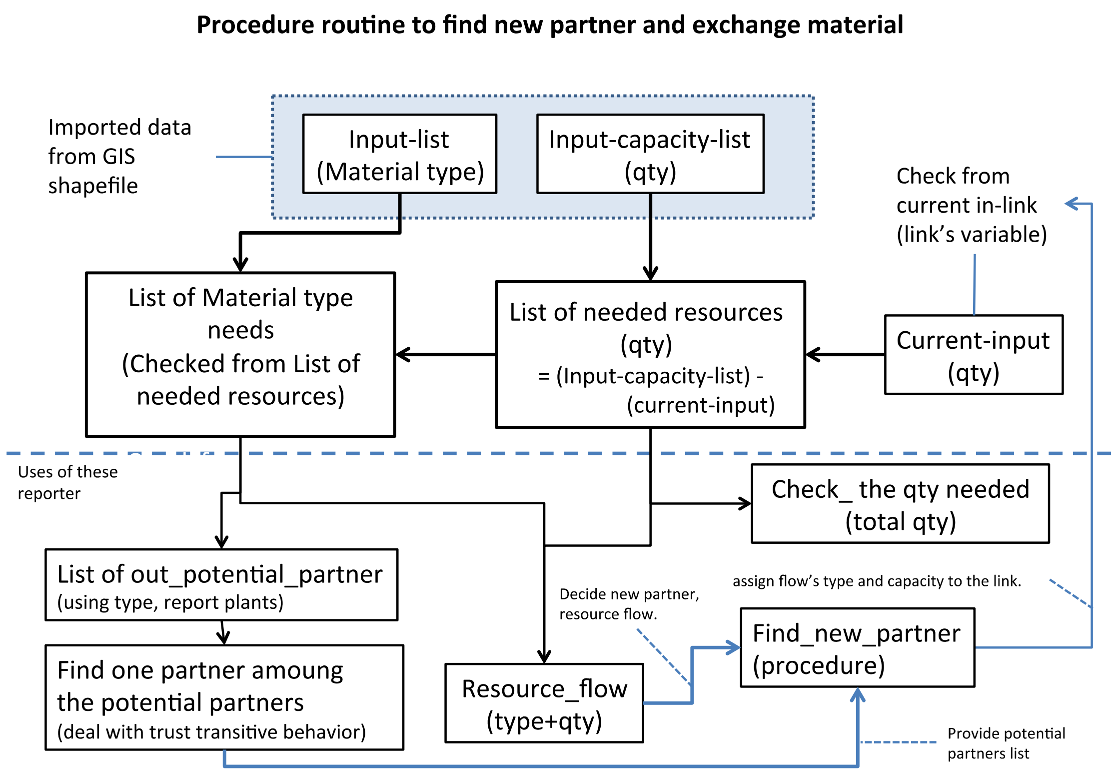


Figure 22: Flowchart of the main procedure: Exchange of material

4.2.3.4 Process overview and scheduling

At every time step, each agent performs the following tasks in a chronological order:

If a pioneer plant:

1. Find a partner for exchange of material; each plant looks for an input, or more, up to the maximum of link set up by the user, among the

output of the other plants. If there is availability of material that correspond to its input a link between the two entities is created, the behavior of the now partnered plant is set to 1.

2. “Hatch” a truck: One material is found, a truck leave the plant of origin with the matching material and send to its destination using the shortest path.

If a follower plant:

- If there are more than 10 partnerships within the network: the follower plant imitates the pioneer’s behavior, which is performing steps 1, 2 and

Both breeds (pioneers and followers):

3. Remember past partnership (use link-memory): If there is availability of input, then the plants use trust transitivity algorithm; if the potential partner has a partner in common then the plant will perform a “preferential” partnership.
4. Learn and imitate the most frequent behavior within a set radius determined by the user.
5. Emit CO_2 during delivery
6. Calculate CO_2 avoided: compare to traditional business to business delivery

4.2.4 Results

4.2.4.1 Model Verification

When constructing such complex models the sensitivity of the main components and parameters should be checked. For this sensitivity analysis the following the main factors of model: Cultural cooperation, Learning ability and effect of a carbon tax will be compared.

On this experiment, the probability of cooperation and the learning ability parameter: TRUE” and “FALSE”, are analyzed. The impact results monitored are on the quantity of by-product exchanged. The goal is to determine if the social learning has a real influence on the symbiosis and for how long, and if the social learning is complementary or competitive to the cultural cooperation algorithm in the model. Figure 23 shows the results regarding the cultural cooperation probability: On a low cooperation level, we observe that the exchange of material tends to have an important impact at the beginning of the simulation and slowly decreases over the rest of the simulation. This is explained by the fact that the novelty of the exchange initiative tends to have a positive effect on the agents in engaging in the network and start exchanging. At high level of cooperation, we observe that naturally the quantity of by-product exchange is at is highest. However, at medium level of cooperation an interesting result of this simulation emerges, we would expect that the overall amount of by-product exchange would be in between the result of low and high level of cooperation, but the results exhibit the lowest amount of exchanges, one explanation would be that cooperation shows distinct effect at extreme level (low and high) but a medium level of cooperation is more subject to variation.

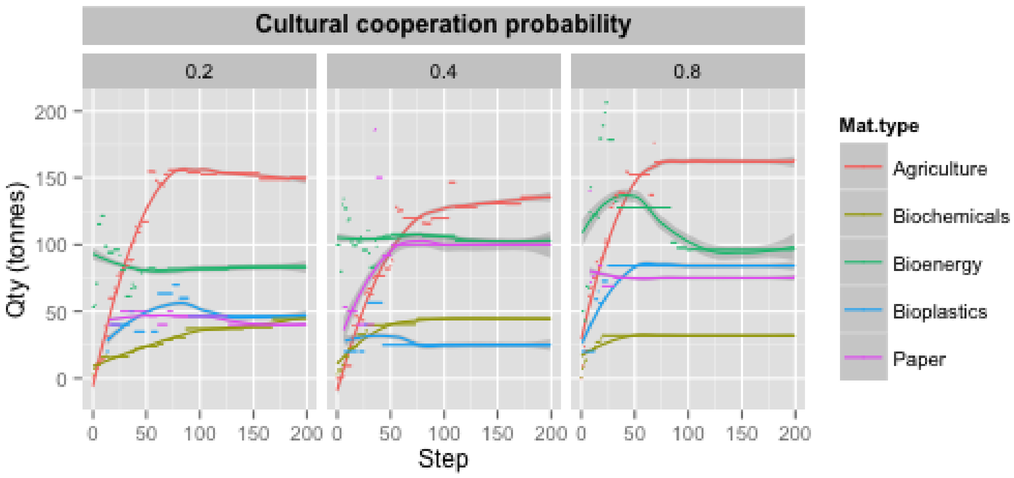


Figure 23: By-product evolution in response of the different level of cultural cooperation

In particular, it was found that there are differences in distribution of the breakdown by by-product. As expected, agriculture by-products are the most important flow in the system, they also are the most stable. Indeed since this EIP initiative revolves around the agro-industry we, not only, expect an abundance of agricultural flow but also that this exhibits the least variations. On the other hand, the bioenergy curve shows some noticeable variation especially at high cooperation level, this is explained by the fact that this flow is being used by a varying number plants, each having much different needs in terms of bioenergy use. Figure 24 shows the results regarding the social learning where other agents imitate the behavior of successful agents. Overall, the experiment results shows expected patterns: higher quantity of exchanges with learning is “TRUE” and lower quantity of exchanges when the learning is “FALSE”.

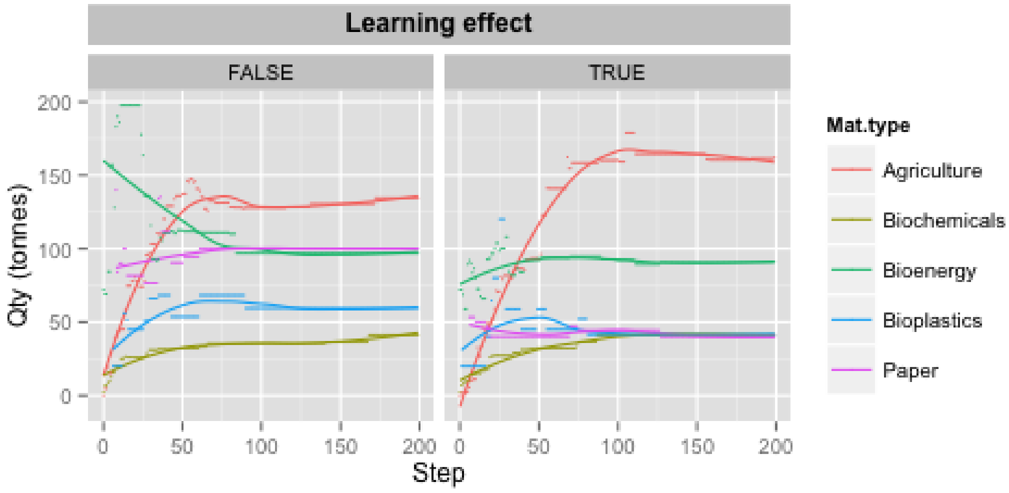


Figure 24: By-product evolution in response of social learning

We also found that the bioenergy is most affected flow of the system: all the other by-product shows differences in quantity but a similar patterns with or without learning. But, just like with the cultural cooperation, the amount of bioenergy by-products exchanged exhibits an interesting behavior by being the only flow exhibiting a steep decline when the agents do not have the opportunity to use the “social learning” algorithm. This could be explained by the fact that biomass is probably the flow that is the most dependent of the upstream industry.

One benefit of the circulation of flow within an EIP is the geographic proximity of the participants [Chertow 2007]. What is taking this AB model to the next level is integration of a GIS layer as an input data. The layer contains information about the geographic location of the participating plants and the roads they can use for the exchanges. At this point, I would like to remind the reader of the agents routine: once they found a partnering agent, the agent expediting the material also sends truck to transport it to its plants destination (Figure 25). At this stage, the distance between plants is recorded and the CO_2 emitted is calculated using data from the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) Life Cycle Model

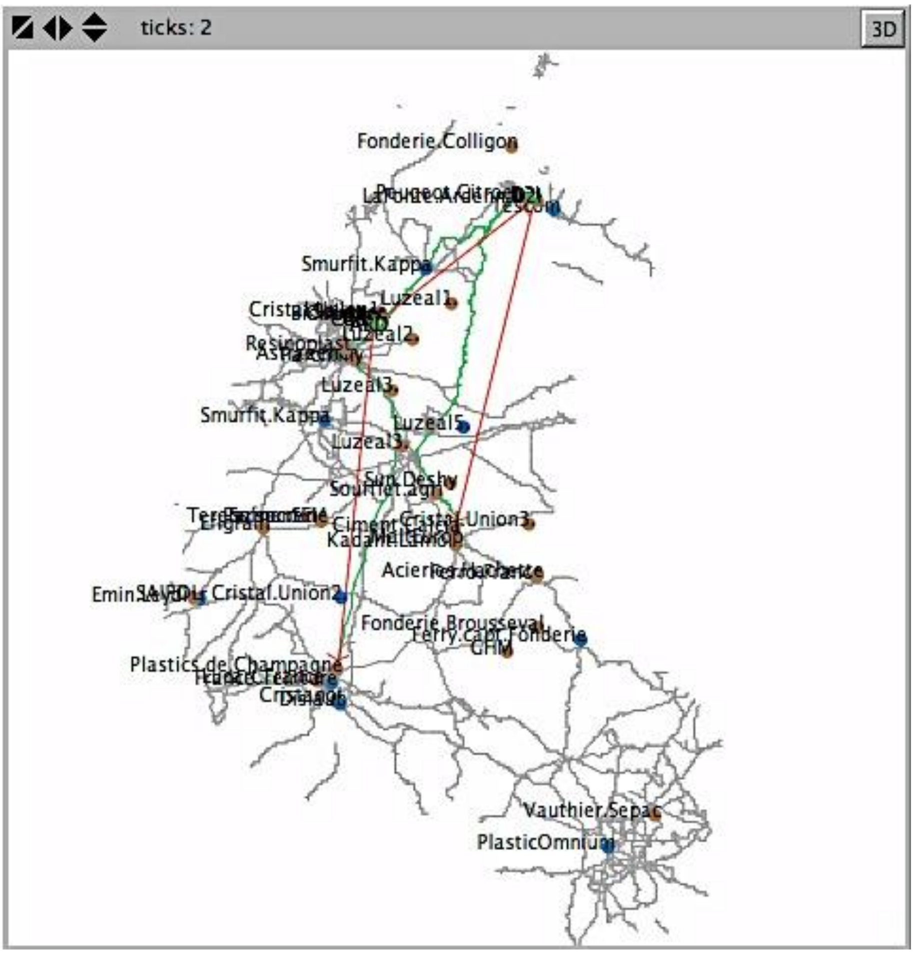


Figure 25: Screenshot of the AB-IS symbiosis on Netlogo.

The red line represents the exchanges of material. The highlighted green path shows the shortest path the truck that transports the by-product.

Figure 26 aims to compare the results of transportation CO_2 emitted during the delivery within the EIP versus the CO_2 that would have been emitted for the transportation of raw material or manufactured inputs from traditional supplier. It is important to note that we hypothesize here that while the distance between the plant in the AB-IS are accurate, the average distance between the plant and traditional supplier is restricted to a random normally distributed random value, which is a simplification of the reality. We also want to know if the social learning and cultural cooperation factor that intervene well at the beginning of the process have an effect on the CO_2 emissions. The results show consistency with the previous experiments results, interestingly while cultural cooperation does not seem to have a direct effect on the amount of CO_2, social learning displays a clear impact on the CO_2 emitted, especially on the amount of Co2 avoided when the industrial symbiosis is in place (blue boxplots). This result confirms what IE advocates have been claiming about IE being an efficient way to reduce CO_2 emissions, it also shows that effort into learning through sharing information and getting engaged in this type of endeavor does have a positive effect the environment.

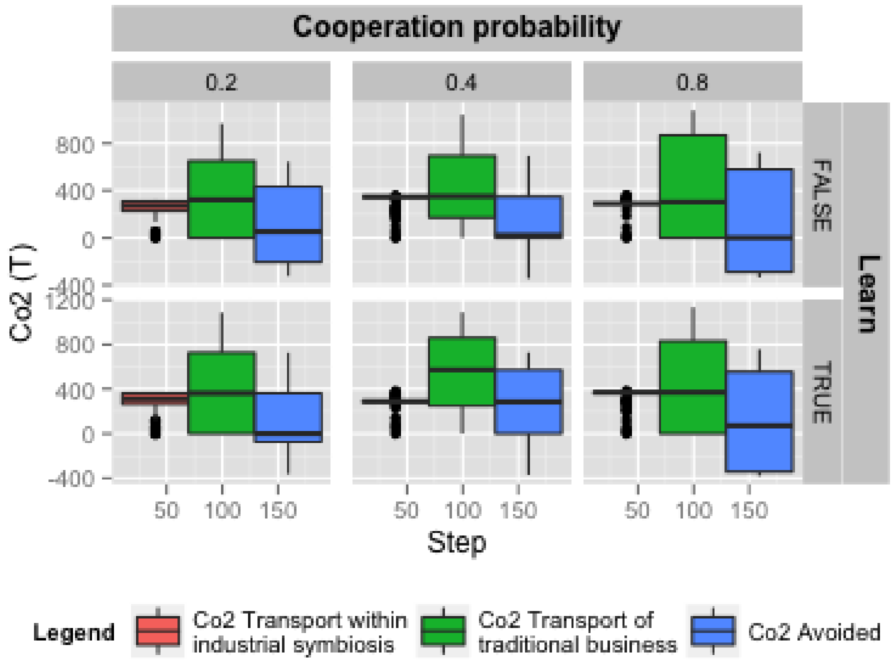


Figure 26: CO_2 emissions distribution during the transport stage of the by-products in response of both cooperation and social learning

4.2.4.2 Model Validation

4.2.4.2.1 Literature comparison

The encoded model needs validation to show if the model is fit-for-purpose. This is a complex task because the model is based on a gross simplification of the real situation and the experimental conditions are necessarily far removed from market and political conditions. For example, the model does not allow for the complex behaviors of a real manager of the supplier who may stop or reduce supplying products to one of the retailers because of some social (for example, boycott) or political (for example, on different sides of the political agenda) issues between them. Verification is a relatively straightforward task, and our model assumptions has been checked and compared to published papers (see articles Ehrenfeld and Gertler 1997a; Heeres et al. 2004) that confirm that this model can be seen as a simplification of reality. Indeed, symbiosis requires not only a large exchange of information about nearby industries and their inputs and outputs, but also about their production processes and logistical organizations. This implies a strong cooperation between entities without which no link can be implemented. Very few studies have been performed on what favors the emergence of industrial symbiosis. However in their article, Ehrenfeld and Gertler (1997b) emphasize that the success of the symbiosis of Kalundborg can be attributed to the fact that the town is a tight-knit rural community of 12, 000 residents, where managers and employees interact socially on a daily basis, resulting in a cultural feature that encompasses a short mental distance between firms. This seems to have triggered the learning from the neighboring firms, who were not initially involved in the symbiosis, but, after " learning" about the concept and the benefit, eventually joined the network.

Also, a review of past Industrial Symbiosis initiatives can be used in order to validate the hypothesis for the model. Indeed, in their article, Heeres et al. [Heeres et al. 2004] compares six cases with an "ideal development process" considering the following aspects:

- "History and location of EIP;
- Stakeholder involvement and project organization structure;
- Planned EIP development (development vision);
- Economic and environmental impact of the project;
- Results (established EIP development up till now, what has been realized?)
- Factors essential to project success and/or failure. The scoring ranges from 1 to 6 for each aspect on which the projects were compared", the best project scored 6 points, the second best 5, third best 4, etc. [Agarwal and Strachan 2006].

Some of the defined measuring aspects chosen by Heeres et al. (2004) are analogous to our own agents and environment characteristics. Indeed, the participation corresponds to our "involvement index". The vision can be linked to the trust and doubt as well as the group categories (pioneers and followers) of our agents. Finally the economic and environmental impact result matches our indicators monitors (Total CO_2 and CO_2 by type of behavior). Heeres and Al. (2004) also identified other factors that contributed to the current success failure of the EIP initiatives (see **Error! Reference source not found.**).

Table 6: Factors essential to the success or failure of the reviewed cases [Heeres et al. 2004] (reproduced)

Factors essential to success or failure of the six cases reviewed		
Project	Factors essential to project success	Factors causing problems or failure
INES	Active participation of companies, environmental management network, Europort employers' Association	-
RiVu	Active participation of companies, Entrepreneurs Association RiVu	Few large, financially strong companies, differences of opinion regarding rezoning of the RiVu industrial park
Moerdijik	Active participation of companies, existing exchanges relationships, entrepreneurs association	Relatively large distance between companies
Fairfield	-	Baltimore and state politics, lack of company interest, absence of an entrepreneurs association that represents all Fairfield industries
Brownsville	-	Lack of finances needed to improve the computer program used to identify possible exchange relationships, lack of company interest
Cape Charles	Active participation of local residents, cooperation between town and county	The attraction of industry to Cape Charles, the location terms demanded from candidate companies

They conclude that active participation as well as cooperation is essential for such projects. Existing exchange relationships being the equivalent of our agent memory of past partnership is also identified as an essential factor for project success. Distance is also identified as a possible obstacle, which is also one of the features of our model. Considering the diversity of EIPs and their geographical context it is difficult to define standards aspect for validation, however some of the reasons for project success and or failure seem to be fairly uniform. Although the actual state of the model shows some of the essential mechanism patterns of symbiosis, which is essential to understanding the emergence of such a system, it does however miss some important aspects that eventually help in reaching the "Medawar zone" of complexity. In order to do so, the following aspects should be included in subsequent versions of the model:

- Reaction to regulatory framework (political, environmental, and social): high or low government intervention as well as strong or more lenient environmental/labor regulations greatly affects even the possibility of implementing a symbiosis. The right dose of regulation should be investigated so the model can become a more replicable one.
- Financial ability to participate for the design and implementation of new infrastructure for the EIP is also identified by Heeres et al. (2004) but had been overlooked for the current version of this model.
- Reaction to regulatory framework (political, environmental, and social): high or low government intervention as well as strong or more lenient environmental/labor regulations greatly affects even the possibility of implementing a symbiosis. The right dose of regulation should be investigated so the model can become a more replicable one.
- The nature of symbiosis itself: some are spontaneous (bottom-up) while others are planned (top-down). This model assumes that symbiosis emerges in a bottom-up fashion. However, some industrial ecologists are investigating the idea that symbiosis can be built from scratch from a Brownfield or an existing industrial cluster. This could be a topic for another model in the field of IE.

In her thesis Yu [Yu 2003] states that EIP implementation is not an "overnight" occurrence, "it is a process that involves interactions among actors nested in the institutional, natural and economic environments….They share knowledge or adopt technologies to reduce pollution depend on certain preconditions and evolutionary mechanisms" [Yu 2003]. Trought a litterature review she summarized this process (Figure 27).

	Stages	Triggers	Outcomes
Three-stage model (Chertow and Ehrenfeld, 2012).	Sprouting	Economic efficiency. Regulatory pressure. Social relationships. Resource security. Supply chains of firms.	Firms begin to randomly exchange resources.
	Uncovering	An actor (e.g., a coordinator or local authority) whose focus is beyond the private transactional network observes and uncovers.	The realization of positive environmental externalities becomes consciously uncovered and pursued.
	Embeddedness and institutionalization	A coordinator engages potential symbiotic partners and strengthens the shared norms which can facilitate more complex exchanges.	Further expansion of the network becomes intentionally driven.
Stages of a facilitated IS network (Paquin and Howard-Grenville, 2012).	Primarily serendipitous processes	Taking strategic view of region's resources. Using pre-existing contacts to engage firms. Facilitating interaction spaces.	Firm's interest is captured and led to broader institutional awareness. Potential exchanges are found through workshops.
	Mix of serendipitous and goal-directed processes	Strategically introducing relevant firms around low-hanging fruit. Deepening involvement with firms and projects.	Deeper relationships, trust are developed. Firms are re-engaged in new exchanges.
	Increasingly goal-directed processes	Replicating high-value exchanges. Developing capacity around key regional resources.	Selected firms increasingly engaged around replicable exchanges. Selected complex projects to support future IS exchanges.
Building trust and embeddedness in the IS development (Doménech and Davies, 2011)	Emergence	Stringent regulations. Limited resources. Policy actors' initiatives. High coordination.	Formation of the network. Some straightforward cooperation opportunities are explored.
	Probation	Learning by doing. Implicit and explicit negotiation and cooperation. Potential IS exchanges are unveiled and tested.	Realization of first IS exchange projects. Generation of dynamics of cooperation and building trust. IS is gradually integrated in the decision-making.
	Development and expansion	Continuous and frequent interaction generates trust and builds a shard vision to develop embeddedness. Learning from past experience and tacit knowledge. Joint problem solving and exchange of fine-grained information assists to identify new IS exchanges.	Deeper embeddedness in the network. Attracting new members and opening up the potential for new exchanges. Diversifying the material and organizational base of the network.

ABM scope

Figure 27: Stages of IS development in the literature

[Chertow and Ehrenfeld 2012; Paquin and Howard-Grenville 2012; Domenech and Davies 2009; Yu 2003].

The AB-IS included the key factors of EIP development: trust and cooperation as agents variable and validate the outcomes hypothesis that "IS is gradually integrated in the decision making" [Yu 2003]. Indeed all verification plots results (Figure 23,

Figure 24 and Figure 28) show that quickly after the beginning of the simulation we observe that the system reach some sort of equilibrium.

Historic replay

The aim of historic replay is to compare our model to the scenario of a real-world scenarios by looking if the behavioral patterns of the model and the state in the real system show similarities. If successful, we can claim a degree of validity by the model [Dam et al. 2012]. The challenge here, is finding data over a reasonable time frame in order to be fit for comparison. In consideration of this issue, we choose to compare our model to the case described by Park et al. 2008: The sustainable development of industrial park in Ulsan, South Korea, a cluster of inter-networking businesses, which perform individual and collective cleaner production program prior to by-products exchange network [Park et al. 2008]. Figure 28, shows the evolution of both symbioses over a period of 10 years. To allow meaningful comparison, we will compare both systems over the same period of time

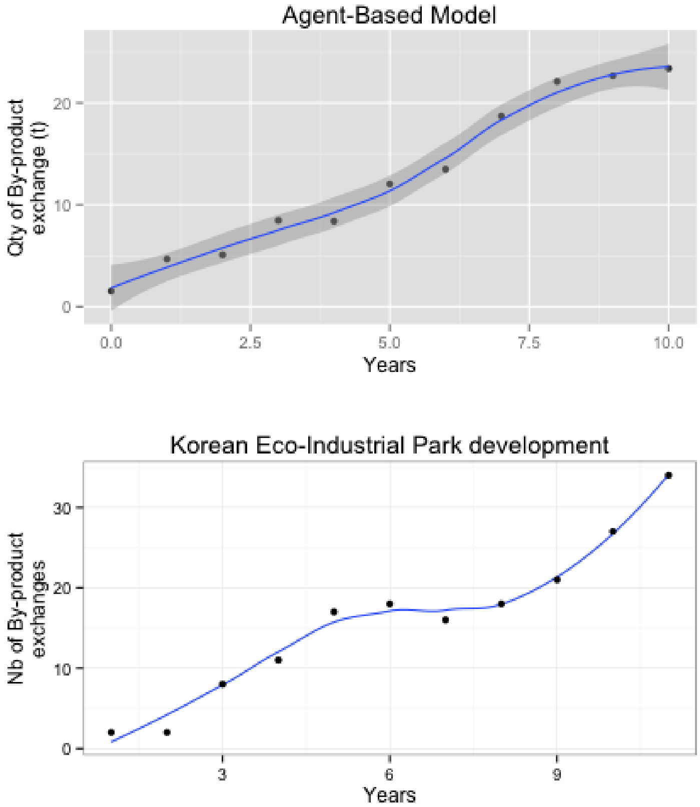


Figure 28: Model comparison between AB-IS and real-world evolution Korean industrial eco-park

Here, we want to determine if both systems exhibit the same evolution pattern. Interestingly, the AB-IS seems to replicate an evolution similar to the real world. We observe a continuous increase in by-product exchange with a slight slow-down after the 5 first years. Although, we cannot expect a perfect match, we can explain the difference in the pattern sharpness where the AB-IS display a smoother pattern, this is mostly due to fact the quantity plotted is an average count of all runs.

Figure 29 shows the actual breakdown by material type. It is interesting to notice that bioenergy derived from the biomass feedstock curve, which represent the main flow in our case study, shows a quasi-identical pattern as the Korean evolution. On the other hand, regarding the rest of the material flow type, they do not display a matching pattern but agriculture and biochemical by-products still show a slight increase over the simulation.

Figure 29: AB-IS By-product exchanges evolution by material type

4.2.5 Summary of the results

The main research question is: What level of endogenous and exogenous factors (cultural cooperation, social learning ability etc.) is necessary for IS development and durability? **Sub-questions derived from the main question are**: Can we identify a balance between the exogenous factors (observed cooperation culture in the region etc.) and the endogenous factors (learning, level of trust and doubt) that would be optimal for IS development? Can these findings be replicated to other regions?

The current state of development of the model shows promising results. Indeed, in this AB-IS case study we presented our initial effort in a simulation model that captured the behavior of heterogeneous agents while adopting a macroscopic approach of the environment.

The results of the selected scenarios show that social learning has more impact on the positive development of the symbiosis than cultural cooperation. In most cases, cooperation seems to be need at the beginning of the simulation, during the first 10 years, in order to multiply exchanges; it then seems to have no more effect on the systems behavior. The learning aspect emerges later during the simulation but has a longer lasting positive effect on the symbiosis development. This model also revealed that individual social learning can show downstream environmental impact over the network. Understanding the specific reasons of these findings will be difficult to analyze at this point, however this explorative model allowed for simulation of a variety of scenarios showing the basic behaviors of such systems, which is seen as an approach to modeling multi-agent network systems that may serve as the basis for the development and sustainability of industrial symbiosis. Adding the GIS layer proved to be useful, indeed we were able to use the actual distance between plants and determine the amount of emissions emitted during the transportation stage. This model provides a basic framework that allows for many interesting extensions:

- Introduce other critical resource impact such as water consumption
- Consider the total benefit from resource exchanges (resource consumption, CO_2 reduction, etc.), maybe add a 3rd agent such as water treatment facilities using GIS data.
- Take the social learning factor beyond the imitation of other agents behavior and past experiences by having them respond to (or anticipate) the effects of an ever-changing social environment and become fully adaptable to each other and their environment.
- Incorporate an information sharing scheme between agents and a regulatory algorithm (carbon-tax, subsidies, regulations)

Finally, in the field of IE, quantitative tools used to assess sustainability, such as LCA, Material Flow Analysis and others, have been subjected to an increasing amount of research. However, there is still a lack of fundamental understanding of how industrial symbiosis emerges from the bottom up in order to establish sustainable systems. Social learning and cultural behavior as well as business norms and practices have been overlooked despite their importance. The consequence of individual behavior on the sustainability of a system is difficult to measure with traditional assessment methods. Ultimately, the greatest use of ABM will be in the generation and exploration of alternative futures and scenarios that may emerge under varying situations. This will show the possible evolutionary patterns of certain scenarios under changing conditions and varying geographical contexts - an industrial eco-park is therefore a relevant area of application.

Chapter 5 Conclusion

The purpose of this thesis was, on the one hand, to explore how the behavioral factors in adopting a new biomass crop impact the environmental life cycle of switchgrass production, and reveal the relevant behavioral factor that promote the development of an EIP around the agro-industry, in order to provide new insights in designing biofuel-focused public policies. On the other hand, the challenge was in using a new methodology, agent-based modeling, in tackling the problem of introducing human agency in informative simulation modeling, and therefore in evaluating the appropriateness of the method. The hybrid approach of LCA and ABM has been explored in this research. This chapter aimed to generalize the approach and it was tested in a different case study. The results, even thought, are not intended to determine exact predictions of environmental impacts, showed the relevance of integrating social variables into LCA modeling and the necessity to integrates the dynamic aspect of the system into the modeling framework. The other modeling approach integrating GIS and ABM also showed promising results. The application of the proposed approach has shown that by adding the spatial relation between plant-agents, data about the environmental and organization impacts of logistics within an EIP can be gather and analyzed. This approach can be used for existing EIP to assess prospective scenarios of investments and potential economic and environmental benefits, particularly important for industrial network that spreads over a large area and involves a large number of participants, which increase the level of complexity.

5.1 Addressing the research question

This research presents and executes a framework for the AB simulation of farmers and plant manager behavior. As an exploratory effort, this research develops an integrative ABM methodology: AB-LCA and AB-IS that, through the external validation, was successful in creating realistic patterns. Building such models poses a significant challenge, which led to the main research question: *What is a suitable modeling approach for sustainable socio-technical systems that allows the user to make social and technical changes in industrial ecosystem and help decision makers to experiment prospective "what-if" scenarios in a* *dynamic, and evolving environment?* Attempting to "capture" the socio-physical aspect of a system, as well as the emergent effect resulting from the aggregation of individual behavior, is a challenging task. The experience of this research effort has demonstrated the need for more flexible and integrative approach in modeling complex adaptive system, particularly the need for modularity in building simulation framework. To do so, we have identified the components of this framework and summarized them in the diagram below:

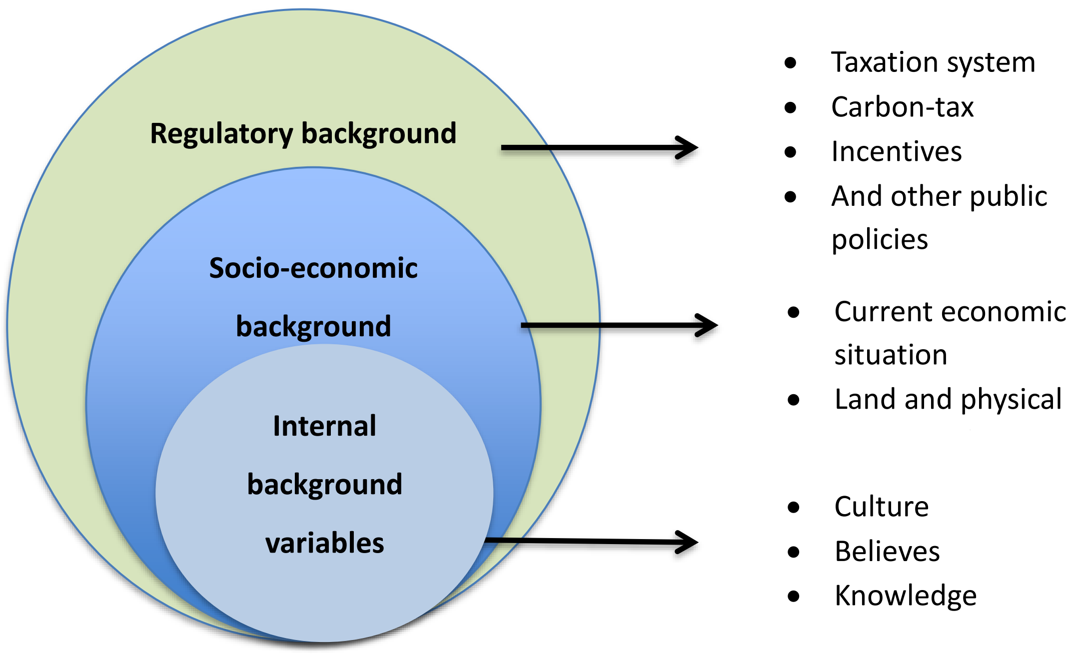


Figure 30: Integrative sustainability model framework

These components are meant to be modular and inter-changeable. Each module forms the interface needed to bring different aspects of the system (both social and physical) together and to interconnect different models. Although not equally addressed, this approach has been demonstrated in our case studies (Chapter 3) by using each of these modules as input variables. In summary, the advantage of this framework is its inter-operability, by allowing the setup of sustainable models of socio-technical systems re-using existing "building blocks" from models developed under this framework and allowing the comparison of different system boundaries scenarios in which the decision makers are modeled.

5.2 Interpretation of findings

This thesis demonstrated the significance of incorporating endogenous factors, that are traditionally left out from other research studies, such familiarity and risk aversion in the first case study and as social learning and cooperation in the second case study, in implementing a modeling framework and the usefulness of using actual data (LCA data and GIS layer) as model inputs. Within both ABM, farmers and plants managers are represented as agents that have individual characteristics and make decisions based on their environment and beliefs. This integrative methodology brought traditional modeling approach to the next level. Indeed, instead of using heterogeneous agents, they usually use a single average entity, which is static in nature. As both models are built bottom-up it does not only enable us to "measure" endogenous and exogenous factors levels at the same time, but to also to begin to understand such results.

In the first case study, we assessed the role of risk-aversion and familiarity as endogenous variables, switchgrass selling price and potential profit as exogenous variable in LCA of switchgrass adoption, we have shown that although endogenous variable have some limited effect on adoption, the greatest contributor in the decision making is the profit expected to be made by selling switchgrass, which confirm assumptions from the literature. But more specifically, we were able to isolate a direct impact of this variable on switchgrass LCA. Another value of AB-LCA model is that as the model is satisfyingly calibrated, in theory, no actual flow measurements are needed as an input and it which unable us to learn about the system before a switchgrass-based ethanol market is in place. This combined LCA-AB model showed to be useful in refining LCA with a theoretical case study by complementing existing LCA model and tackling uncertainties in the techno-system that result from unexpected user behavior. The model can be extended with regards to the scale of complexity that we want to explore. A GIS extension with real life parcels, using actual yields and roads for transportation to the refinery can be added. Although this model is developed using decision-making scale at household level, but the main purpose is to explore emergent behavior at larger scale, how the majority adopts certain land use system.

In the second case study, we explored how significant social learning and cultural cooperation is to EIP implementation. Indeed, it has been oberserved in empirical research that EIP plannning project often suffers from misunderstanding of the local context and lack of enforcement. Therefore capturing and understanding the endegenous factor that influence EIP implementation are essential. This combined AB-GIS model, using real life plants, some of them being already engaged in a a local industrial symbiosis initiative, is an advancement by itself. In this model, we have shown that social learning is most determinant factor in EIP implementation and development. This means that efforts in information sharing, trainning and promotion have to be a priority in EIP planning. Although, significant variable such as the economic aspect of the exchange had been left out, results of the external validation of this model showing similar development pattern gives us some confidence about its calibration. Further version of this model should include price value to the exchange and measure economic savings.

5.3 Limitations and Recommendations for further research

These concluding remarks would be incomplete if we did not mention several important limitations of our model and results. Both models need to provide useful information and we should feel confident about what the results revealed. As I. Nikolic put it: Model validation is a continuous process [Nikolic and Dijkema 2010] these models are far from telling us everything we need to know, however, there initial design to give the attempt insight in agent behavior in eco-industrial system.

Aside from the fact that AB modeling has its inherent limitations, both models were restricted to a limited number of assumptions and data availability, which definitely can easily take the model one direction to an other. Nevertheless, both models were used as “what if “ scenarios to compare relative outcome differences across change in parameters and their results when compared to the broader literature are generally consistent. Having said that, these models cannot be used as realistic to be directly used for system development without validation of both models through stakeholder interviews and participation, who have the best knowledge of the system. This would be a great point of improvements to make these models as templates for sustainable system development. Finally, there still remains a methodological question about the shape of tools that should be developed to modeling human decision-making and behavior in sustainable industrial eco-system. While this thesis shows one such implementation, it is not the only one, and the ideas presented here can be remixed into other implementation.

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