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6 7 8 **A Stochastic Approach to Model Dynamic Systems in LCA**

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15 **Keywords:** Bayes Theorem, technology diffusion, switchgrass, agent-based modeling,
16 emerging systems, social networks

17 18 19 **<heading level 1> Summary**

20
21 This paper presents a framework to evaluate emerging systems in life cycle assessment
22 (LCA). Current LCA methods are effective for established systems; however, lack of
23 data often inhibits robust analysis of future products or processes that may benefit the
24 most from life cycle information. In many cases, the life cycle inventory (LCI) of a
25 system can change depending on its development pathway. Modeling emerging systems
26 allows insights into probable trends and a greater understanding of the effect of future
27 scenarios on LCA results. The proposed framework uses Bayesian probabilities to model
28 technology adoption. The method presents a unique approach to modeling system
29 evolution and can be used independently or within the context of an agent-based model
30 (ABM). LCA can be made more robust and dynamic by using this framework to couple
31 scenario modeling with life cycle data, analyzing the effect of decision-making patterns
32 over time. Potential uses include examining the changing urban metabolism of growing
33 cities, understanding development of renewable energy technologies, identifying
34 transformations in material flows over space and time, and forecasting industrial

1 networks for developing products. A switchgrass-to-energy case demonstrates the
2 approach.

3 <heading level 1> Introduction

4 Life cycle assessments (LCA) can have the greatest impact on systems that are
5 not fully developed; however, traditional LCA methods are not yet sufficiently robust to
6 model their complex, dynamic, and emerging nature. The way in which a system evolves,
7 its path dependence, and the types of actors participating in the supply chain may have a
8 profound effect on its environmental impacts (Nikolic and Dijkema, 2010). An LCA of
9 an emerging system may suggest important options for improvement before the system
10 fully develops. By using models that provide insights into potential development
11 pathways, LCA can estimate the environmental impact of a range of future scenarios.
12 These scenarios can identify alternatives that have the greatest potential for improvement
13 and suggest policy options that could lead to preferred outcomes. Kempener and
14 colleagues showed that development pathways influence economic, social, and
15 environmental performance of emerging bioenergy systems (Kempener et al 2009).
16 Despite the uncertainty and analytical challenges posed by modeling emerging systems, it
17 is recognized that foresighting methods can provide valuable information that can be used
18 to identify trends and reduce the probability of unforeseen negative events (National
19 Research Council 2001). The industrial ecology community has also identified research
20 needs in the area of dynamic systems modeling within LCA (Reap et al. 2008, Thomas et
21 al. 2003).

22 In an emerging system, there are many uncertainties regarding the development of
23 a system and its future environmental impacts. In the absence of data, the Inventory
24 Analysis phase of an LCA cannot be completed. In order to obtain relevant information
25 for an emerging system, scenario modeling is needed to simulate plausible sets of
26 inventory data. A number of methods for scenario modeling have been proposed for
27 analyzing future systems in LCA. These methods tend to fall into one of three categories:
28 trend analysis, scenario-based, and agent-based models. Trend analysis extrapolates
29 existing data to a future state. It may be used when systems are expected to develop in a
30 predictable and consistent manner. The major disadvantage is that trend extrapolation

may not reflect reality or capture system complexity (Wenzel 1998). Scenario-based methods, sometimes called prospective LCA (Walser et al. 2011), form either what-if or cornerstone scenarios in an effort to model potential future outcomes (Fukushima & Hirao 2002, Pesonen et al. 2000, Spielmann 2005). Agent-based models (ABMs) use individual decisions to inform how the aggregate system will emerge. ABMs have been used in conjunction with LCA in the past and coupling ABM to LCA is growing in popularity (Halog and Manik, 2011).

A Stochastic Approach to Model Emerging Systems

This paper proposes a stochastic method that falls between proposing what-if scenarios and creating a complex ABM. Bayesian statistics are used to model the probabilistic behavior of potential technology adopters within a system. The approach is intended to be informative rather than predictive, generating numerous plausible scenarios that can have significantly different environmental outcomes. The approach is applicable to any system in which the type of individual or firm adopting a technology may significantly influence LCA results. As an example, consider two types of potential adopters: urban agents and rural agents. Both types of agents are considering a hypothetical technology that emits large quantities of volatile organic compounds (VOC) during the use phase. The quantity of VOC emissions emitted by an urban adopter and a rural adopter are identical; however, the environmental impact of the technology will depend on the geographic distribution of adoption due to higher population densities and greater smog formation potential in urban areas. In this way, the model can analyze how adoption behavior of different divisions of agents affect overall environmental impacts of a system.

This model can also be used to describe future scenarios where the extent of market penetration may impact LCA results. For example, the overall market penetration of natural gas vehicles may have a significant effect on the life cycle inventory of natural gas production. The aggregate effect of individual vehicle purchasing decisions could increase demand for natural gas and shift the supply chain of natural gas. Exploitation of shale and other non-traditional methods could become more common, which have different upstream impacts than the current natural gas supply chain (Jaramillo et al., 2007).

1 The proposed framework can be used as a stand-alone model or as a method to
2 simulate behavior of potential technology adopters within a larger ABM. In ABM,
3 individual agents are assigned rules of behavior and allowed to interact within a
4 prescribed environment. ABM aggregates the microscale interactions of these agents to
5 describe overall system emergence. Insights gained from ABM can be particularly useful
6 for informing policy decisions to achieve a desired outcome. Researchers use ABM to
7 model and predict system dynamics in fields ranging from economics to ecology to
8 transportation logistics (Arthur 2006, Garcia 2005, Grimm et al. 2005). ABM has
9 become increasingly common in the industrial ecology community (Andrews and
10 DeVault 2009, Ashton 2008, Axtell et al. 2001). Davis and colleagues have outlined a
11 specific strategy to integrate ABM into LCA (Davis et al. 2009). In Davis' approach, an
12 ABM is used to grow the system and model its evolution. This data infrastructure is then
13 connected to life cycle inventory (LCI) information. As the agents make decisions within
14 the model, the supply chain of the product changes, which in turn affects the inventory.
15 As the system evolves, the LCI also changes.

16 This paper proposes Bayes Theorem as a mechanism to model decisions among
17 potential technology adopters. The general approach uses a construct similar to Davis
18 and colleagues. Both methods seek to generate plausible future scenarios to determine
19 the the impact of different system evolution on LCA. Also similar to Davis and
20 colleagues, the proposed method overlays LCI information to the data infrastructure
21 created through the modeling method. The main difference between the two approaches
22 is their scope. Davis' model maps different classes of agents and their respective
23 interactions throughout an entire supply chain. The proposed approach is limited to one
24 class of agents, defined as potential adopters of a technology. The obvious consequence
25 of focusing solely on potential technology adopters is the lack of model interactions
26 among different classes of agents (e.g. producers, consumers, regulatory agents) within a
27 supply chain and resultant loss of supply and demand market dynamics. The subsequent
28 advantages of the limited scope are the reasonably straightforward and transparent model
29 equations and the ability to use software familiar to most practitioners (e.g. MatLab,
30 Excel). Therefore, the proposed framework can be used as a stand-alone method if
31 technology adoption patterns are assumed to have the most significant impact on an LCA.

1 If this assumption is not valid, the proposed framework can be complementary to that
2 proposed by Davis and colleagues by acting as a statistical framework that can inform
3 calculation of agent behavior in the context of a larger ABM.

4 It should be emphasized that the presented framework cannot be used in a predictive
5 capacity. Instead, it is intended to explore probable future adoption patterns and the
6 resultant impact on the LCA of a product or process.

8 <heading level 2> *Using Bayes Theorem to Estimate the Probability of Decisions*

9 In the proposed framework, Bayes Theorem is used to describe how individual
10 agents make decisions. Bayes uses prior information about a system to determine the
11 probability of a certain outcome. Bayesian statistics are often used to quantify and
12 reduce uncertainty and have been used previously for that purpose by industrial
13 ecologists (Lo et al. 2005). Bayes has also been used to determine the probability of some
14 future event, such as setting gambling odds, informing decision making, and determining
15 the likelihood of an individual to make a given decision (Loeffenholz et al, 2009,
16 Charness et al, 2007). This framework uses the latter context.

17 Bayes' Theorem calculates the probability of an event, S , given a characteristic or
18 attribute, X . In this model, S is defined as the decision to adopt a new technology. The
19 generic form of Bayes' Theorem is given in Equation 1:

$$\text{Eq. 1} \quad p(S|X) = \frac{p(X|S) * p(S)}{p(X)}$$

21 The goal of the model is to calculate $p(S|X)$ for each potential adopter, which is
22 the probability that an agent with attribute X will adopt the technology S . The attribute X
23 can represent any attribute that influences the decision making process. Agents with
24 different attributes are expected to have different adoption probabilities, and multiple
25 attributes can be assigned to each agent. These probabilities are used to estimate
26 technology adoption and market penetration over time, and the resulting scenarios are
27 used to inform the life cycle inventory. The term $p(X|S)$ is the likelihood that an agent

who has adopted the technology possesses attribute X . Further, the probability $p(X)$ is the frequency with which attribute X occurs in the population, regardless of whether technology S has been adopted. The ratio $p(X|S)/p(X)$ is a measure of the importance of attribute X for influencing the decision to adopt S . If this ratio is greater than one, the attribute X enhances the probability of adoption; a ratio below one decreases the probability (Lindley 1991). A basic primer on the use of Bayes Theorem is given in the Supporting information.

Equation 1 can be expanded to Equation 2 to show how Bayes Theorem can describe the probability of technology adoption by agents with a specific attribute, X .

$$\text{Eq.2} \quad \frac{\# \text{ adopters w/ attribute } X}{\# \text{ agents w/ attribute } X} = \frac{\frac{\# \text{ adopters w/ attribute } X}{\# \text{ adopters}}}{\frac{\# \text{ agents w/ attribute } X}{\text{total \# agents}}} * \frac{\# \text{ adopters}}{\text{total \# agents}}$$

<heading level 1> **Model Overview**

Figure 1 shows the basic framework of the model. First, agents are classified according to baseline characteristics and decision attributes. Next, the model calculates scenarios that indicate which agents adopt the technology over time. Finally, the results from the iterations are combined with LCI information. An aggregate LCA is compiled, determining the relative contribution of each adoption pathway to the aggregate environmental impacts of the system. Any LCI information that may influence subsequent decisions by the agents is fed back into the decision process to be used in the next time step. The results of a model run indicate how LCA results change according to different adoption pathways over time.

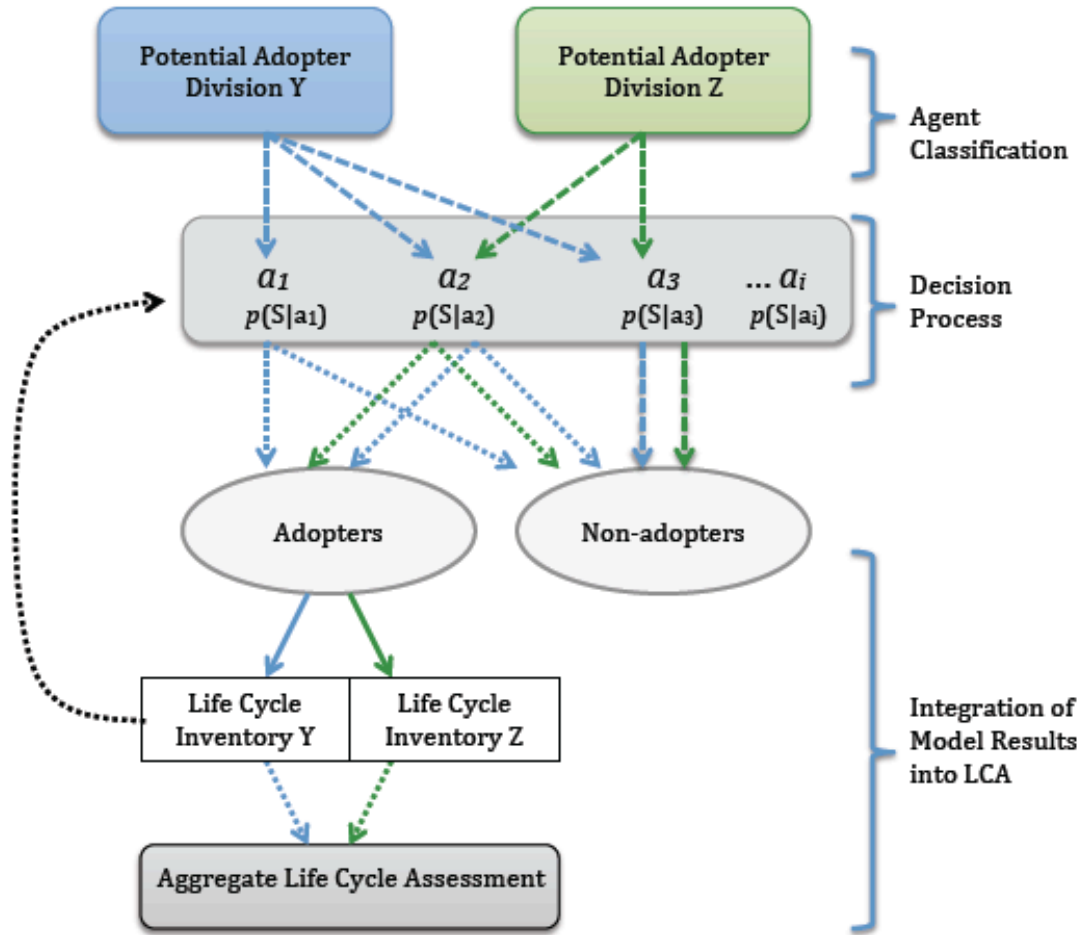


Figure 1. The framework for integrating the stochastic model into LCA. Each agent is classified into an attribute category, a_i . Each attribute category has a probability of adoption, $p(S|a_i)$. Life cycle inventory information is compiled according to the proportion of adopters having different baseline characteristics.

The specific steps for implementing the framework are:

- 1) **Scenario Definition:** Define the scope of the LCA and the necessary parameters for creating the scenario model. Specify the time scale at which decisions are made, including the time step for the simulation, and the total time period over which the system will be modeled. If the defined attributes include a spatial component, determine relevant geographic characteristics of the region.

2) **Agent Classification:** Define the relevant adopter divisions and decision attributes. Each division represents a specific baseline characteristic that is expected to have an effect on aggregate LCA results. Adopter divisions are defined according to state variables that dictate inventory results (e.g. urban and rural agents; owners of active cropland and owners of marginal land), whereas decision attributes dictate decision behavior (e.g. resistance to change). When multiple decision attributes exist, all possible combinations are included, and each combination of attributes form an attribute category, a_i . Next, the number of agents belonging to each division and attribute category are determined. The attribute categories are not exclusive and may contain agents from multiple divisions.

3) **Decision Process:**

a. ***Initialize the Model:*** Calculate the adoption probabilities for each attribute category, $p(S|a_i)$.

b. ***Run the Model:***

i. *Calculate the number of technology adopters in time step, t :* For each agent, draw a random number q between 0 and 1 from a uniform distribution. If $q < p(S|a_i)$, the agent adopts the new technology.

ii. *Update populations of agents in each attribute category:* Introduce any new information into the system, such as the number and location of technology adopters or changes to the market. Determine whether any agents migrate to a new attribute category given the changes to the model.

iii. *Determine whether any $p(S|a_i)$ changes for the next timestep, $t+1$:* Determine whether any of the initially calculated $p(S|a_i)$ have changed due to external factors. In most cases, these probabilities will remain constant throughout entire simulation despite the fact that agents may switch between adopter classes.

4) **Integration of Scenario Results into LCA:**

- a. ***Determine aggregate system outcomes.*** Calculate an LCI for each potential adoption pathway. Use the scenario results to determine the number and type of adopters that adopted the technology. Create an aggregate system LCI given the percent contribution of each adoption pathway.
- b. ***Integrate relevant LCI into Decision Process.*** If agents' decisions are assumed to be influenced by LCI results, the LCI determined in 4b will be incorporated into the next timestep.

5) **Repeat Steps 3-4 until a desired endpoint is reached.** The desired endpoint should be defined in Step 1, and may be a specific number of iterations or until steady state is achieved.

Standard mathematical software such as MATLAB or Excel can be used as the primary interface for the model. If land use change or other spatial information is necessary to appropriately analyze the system, these platforms can be integrated with appropriate geographic information system (GIS) software.

<heading level 1> **Switchgrass Bioenergy as a Case Study**

Switchgrass provides an ideal example for demonstrating the proposed framework. An energy crop promoted by the US Department of Agriculture and Department of Energy, switchgrass is a native perennial grass that has never been cultivated for profit (USDA, 2010). The types of landowners who choose to adopt switchgrass may have a profound impact on LCA results since the LCI of switchgrass is highly dependent on previous land use. For example, adoption of switchgrass on a prior cotton field reduces direct emissions of fertilizers and pesticides, reduces upstream emissions of agricultural inputs due to lower application rates, and sequesters carbon by increasing soil organic matter (Chamberlain & Miller 2011). Growing switchgrass on marginal land containing unmanaged grasses or trees has different environmental effects. When undisturbed land is tilled, there is an initial spike in nutrient and sediment emissions in the first years of establishment, as well as a “carbon debt” that occurs when

soil organic matter is oxidized before being rebuild in soils (Chamberlain & Miller 2011, Gelfand et al 2011). If indirect land use change is taken into account, the effects of previous land use are even more pronounced since producing bioenergy crops on marginal and actively managed agricultural land have different market displacement effects. Therefore, the environmental impacts of switchgrass bioenergy depend largely on whether cotton farmers or owners of marginal land choose to adopt switchgrass. Aggregate LCA results change depending on the extent to which owners of cotton and marginal lands adopt switchgrass.

This section uses potential switchgrass adoption to show a demonstration of the proposed framework among different types of landowners. Representative parameter approximations are used in this paper rather than site-specific data and the resulting simulation results should not be used to infer actual adoption probabilities.

<heading level 2> ***Step 1: Scenario Definition***

The choices made within the traditional LCA scoping process must still occur using this scenario model. The resulting scenarios define the location, extent, and prior land use where switchgrass is adopted, which is then linked to LCI information. Given assumed switchgrass yields and ethanol conversion factors, the area of adopted land is converted into MJ of ethanol or other appropriate functional unit. The framework can be used to inform both attributional and consequential LCA. The effects of the scenarios will be more pronounced in consequential LCA where displacement effects of land use change patterns are taken into account. Attributional LCA will also be affected since there are distinctly different annual biogeochemical fluxes that result from different direct land use change patterns.

Time steps may be defined for any appropriate period (e.g annually, quarterly, daily). The model is run for a defined number of time steps or until it reaches equilibrium. For the switchgrass case, an annual time step is chosen since management decisions regarding crop selection are discrete and occur yearly. The simulation is set for a 20-year timeframe. Once a landowner decides to adopt switchgrass, it is assumed the field remains in switchgrass throughout the model run.

< heading level 2> **Step 2: Agent Classification**

All agents in the switchgrass example are landowners who have the potential to adopt switchgrass. Adopter divisions are assigned according to current land type, since previous land use is the major baseline characteristic assumed to have an effect on the switchgrass bioenergy life cycle inventory. The two major types of land use are actively managed agriculture and marginal land.

Next, decision attributes are chosen. For the switchgrass case study, three attributes are expected to influence adoption of a new technology. These attributes are an individual's resistance to change (R), profitability (P), and familiarity with the technology (F). For other systems, additional or alternate attributes may be chosen as needed to capture system-specific factors influencing decision-making; however, it is expected that these three attributes represent a reasonable starting point to address many systems.

The resistance attribute (R) reflects the willingness of individuals to adopt new technologies and is split into three classes: early (r_E), moderate (r_M), and resistant (r_R) adopters. Note that this attribute reflects the personality of an individual or agent. It is not a measure of the maturity or pervasiveness of a technology, how familiar the adopter is with the technology, or economic factors that influence a decision. Each of these attributes influences decision-making independently. Resistance attributes are distributed randomly to agents according to the percent of the population assumed to be early, moderate, and resistant adopters based on demographic information (Sundling & Zilberman 2001).

The second attribute, profitability (P), is defined as the difference in profits of technology adoption relative to the baseline. For this generic model, three classes are identified: low, medium, and high (p_L, p_M, p_H). Specific ranges for these categories can be determined based on the system. An agent is highly unlikely to adopt a technology that will reduce profitability. Therefore, many systems will benefit from inclusion of a null probability category, p_{np} , which assigns a zero probability of adoption due to economic infeasibility, or $p(p_{np}|S)=0$. Although agents within the null probability category may be

1 excluded from the model, this is not recommended. An initially unfavorable economic
2 decision may become feasible as market conditions change. Agents with an initial
3 adoption probability of zero may migrate into alternate profitability categories over time.
4 For simplicity of presentation, the switchgrass case study assumes that only agents that
5 have the potential to make a profit from technology adoption are included within the
6 model.

7 Finally, decisions are also assumed to be influenced by an agent's familiarity with
8 a new technology (F). As a technology becomes proven and adopted by peers, agents
9 become more willing to adopt it (Rogers 2003). Therefore, as familiarity increases, so
10 will the probability of adoption. This dynamic attribute is a fundamentally different and
11 independent attribute from resistance (R), which is expected to be static as it reflects a
12 willingness to embrace change and is a manifestation of an agent's personality.
13 Familiarity is also split into three categories: low (f_L), medium (f_M), and high (f_H). F
14 depends on the pervasiveness of the technology and the ability to learn about it through a
15 social network. Social networks are often difficult to quantify. Although spatial
16 proximity is often an indicator of familiarity, supply chain or other information networks
17 may also be used (Conley & Udry 2001, Valente 1996). Familiarity classifications will
18 change over time. In geographically relevant systems, GIS may be used to determine
19 changes in familiarity by calculating spatial proximity to other technology adopters.

20 The agents are then assigned to attribute categories, a_i , where the subscript i
21 denotes a particular combination of the attributes R , P , and F . For example, if attribute
22 class $i=1$ represents the combination of early adopters (r_E), high profitability (p_H), and
23 high familiarity (f_H), then the probability of this attribute class will be denoted as:
24 $p(A=a_1) = p(R=r_E, P=p_H, F=f_H)$ or simply as $p(a_1)=p(r_E, p_H, f_H)$. Given that we split each of
25 our three attributes R , P , and F each into three divisions, there are 27 possible
26 combinations of attribute classes, a_i . Any agent within the model is assigned to one of
27 these 27 classes. Although not included in the switchgrass case study, a null category, p_{np} ,
28 included for economically unviable participants will result in 36 categories. The nine
29 attribute classes that include p_{np} will automatically have $p(S|a_i)=0$.

Probabilities for each of the attribute classes can be determined using system specific information. For the switchgrass case study, information regarding resistance to change (R) is available for the general and farmer populations from sociological studies (Hipple & Duffy 2002, Jensen et al. 2007, Ridgeley & Bush 1992, Rogers 1995, Saltiel et al. 1994, Thomas et al. 1990, Vander Mey 2004). In the case of switchgrass adoption, farmers tend to be a community fairly resistant to change, and so the resistant adopter class is larger than most communities (Feder 1980). Profitability (P) can be determined by the current land use relative to what the agent could make with switchgrass. Current crop type is assigned based on the acreage of each crop grown per county and can be obtained through the US Agricultural Census (USDA 2007). Profitability classifications may change over time according to shifts in commodity prices of switchgrass relative to other crops. Familiarity (F) is determined using spatial proximity. Landowners belong to a defined region with a 50-mile radius. The 50-mile radius corresponds to an average extension agent's territory, and is expected to be the basis of the social network (Warner 2008). As the number of farmers growing switchgrass within a region exceeds a threshold value, the familiarity of other landowners in that region increases.

<heading level 2> **Step 3: Decision Process**

<heading level 3> *Step 3a: Initializing the Model*

The inference of the 27 probabilities for each of the attribute categories, i.e., $p(S|a_i)$ for $i=1$ to 27, is necessary to initialize the model and set the baseline. In order to calculate the decision probabilities, Equation 3 can be derived from Bayes' Theorem if mutual independence of the three attributes can be assumed (Lindley 1991).

$$\text{Eq. 3} \quad p(S|a_i) = p(S|r_x, p_y, f_z) = \frac{p(r_x|S)}{p(r_x)} * \frac{p(p_y|S)}{p(p_y)} * \frac{p(f_z|S)}{p(f_z)} * p(S)$$

The defined attributes are assumed to function independently, as there are no obvious correlations between the three variables. Although a high profit potential may influence an otherwise resistant individual to adopt a technology, resistance to change is considered a personality trait that is inherent in the individual, whereas profit potential results from market conditions. If the defined attributes cannot be articulated

1 independently, the basic framework can still be used; however, Equation 3 is no longer
2 valid and the calculations become more complicated.

3 It is assumed that only major changes to the system, such as shifts in cultural
4 priorities or mandated legislation will require recalculation of the 27 probabilities, $p(S|a_i)$
5 initially calculated in this step. Otherwise, the factors influencing individual decision-
6 making are assumed to be stable over time. As the system evolves over each time step,
7 individual agents may switch between attribute categories. For example, an agent may
8 become more familiar with a technology, which will shift that agent into a higher
9 familiarity category with a higher probability of adoption. Market fluctuations may also
10 affect an agent's profitability as the system evolves, resulting in reassignment to a
11 different profitability category.

12 <heading level 3> *Step 3b: Running the Model*

13 To demonstrate the model, a generic simulation for the switchgrass case study is
14 shown. The model code that generated the example figures is available by contacting the
15 authors. A full description of model assumptions and probability calculations for an
16 actual region-specific switchgrass study will be made available in a forthcoming
17 publication, since the derivation, justification, and validation of actual probability
18 distributions is complicated and extensive.

19 For the switchgrass simulation, a uniform grid consisting of 2500 landowners was
20 chosen. For simplicity, switchgrass is assumed to be economically viable for all
21 landowners in the simulation, so the null probability adoption categories are ignored. The
22 model is run for the five scenarios given in Table 1. The simulations provide a simple,
23 but illustrative example for how the model can be applied to help a decision maker assess
24 the effect of different policy instruments meant to encourage switchgrass adoption on the
25 long-term growing patterns within a region. Scenario 1 provides a baseline simulation
26 where no policy instruments are applied and serves as a reference against which the other
27 scenarios can be compared. Scenario 2 considers implementation of a policy affecting
28 profitability for half of the landowners in the region. Scenarios 3-5 demonstrate how
29 different choices for the geographic distribution of demonstration farms affect adoption

1 patterns. Resistance is the same in all scenarios since it is not expected that an
 2 individual's inherent resistance to change can be altered by policy levers.

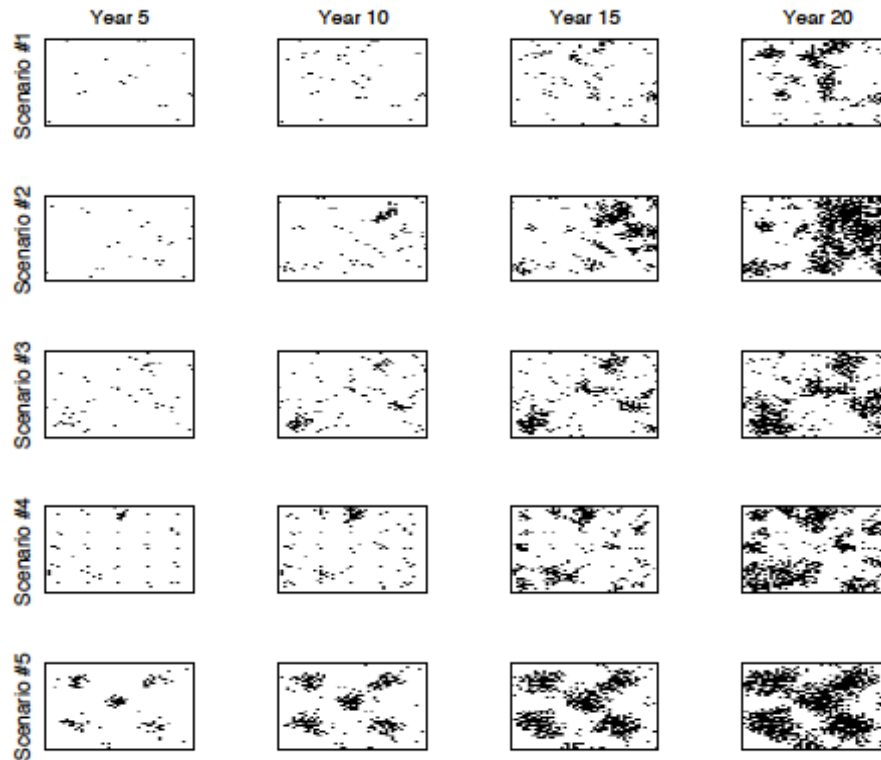
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Scenario	Description	Assumptions
#1	Baseline	At $t=0$, no switchgrass is grown in the system. Familiarity with switchgrass is universally low. Most landowners are within the low profitability category. Resistance is assumed to be typical to other technology diffusion patterns.
#2	Profit Incentive	The region is divided into two equal areas. Region A retains the same adoption categories as the Baseline case. Region B offers an economic incentive to grow switchgrass, increasing profitability classes for landowners in Region B. All other assumptions are the same as the baseline case.
#3	Seed Farms (random)	At $t=0$, 50 switchgrass growers are "seeded" randomly throughout the region. Familiarity of a landowner increases when nearby landowners convert to switchgrass. Profitability and resistance are similar to baseline case.
#4	Seed Farms (uniform grid)	At $t=0$, 50 switchgrass growers are "seeded" in a uniform grid throughout the region. Familiarity of a landowner increases when nearby landowners convert to switchgrass. Profitability and resistance are similar to baseline case.
#5	Seed Farms (regional)	At $t=0$, 50 switchgrass growers are "seeded" in five clusters of ten farmers. Familiarity of a landowner increases when nearby landowners convert to switchgrass. Profitability and resistance are similar to baseline case.

4 **Table 1. Model scenario descriptions**

5 Figure 2 shows a visual progression of a typical run under each scenario. In any given
 6 year, a certain number of landowners convert to switchgrass, indicated by a single black
 7 dot in the grid. To determine which farmers convert in a given year, a random number is
 8 drawn for each farmer. If the number is less than the farmer's $p(S|P,R,F)$, the landowner
 9 adopts switchgrass. If the number is greater, the farmer does not adopt. After any
 10 switchgrass conversions take place, attribute categories are reassigned at the beginning of
 11 the next time step to take into account any new familiarity information. The process is
 12 then repeated to show how landowners may adopt switchgrass over time. Market

1 changes can also be added to determine the effect on adoption, but are not included in
2 this demonstration.



3

4 Figure 2. Schematic showing a spatial representation of model progression of switchgrass adoption over
5 time for five different scenarios (rows 1-5) at $t = 5, 10, 15$, and 20 years (columns 1-4). Black dots indicate
6 a landowner that has adopted switchgrass.

7

8 As the simulation continues, switchgrass spreads to a larger number of agents as
9 agents become increasingly familiar. The model is therefore constructed in such a way
10 that all landowners who stand to increase their profits by adopting switchgrass will
11 eventually convert; however, the model dynamics will determine how rapidly technology
12 penetration will take place and whether a saturation point will be obtained within the
13 timeframe set forth by current bioenergy goals. The system can be made increasing
14 complex by allowing landowners to convert from switchgrass to another crop once they
15 have adopted it. Given that switchgrass is a perennial that requires two years to establish,
16 that possibility is excluded from this model since conversion to prior management
17 schemes is unlikely in the short term.

Figure 3 shows cumulative adoption behavior for the demonstration model under each scenario. Solid lines show the mean adoption curve of twenty model runs, and dashed lines show one standard deviation of these results. The resulting adopter curves display the S-shaped curve typical in technology diffusion (Rogers 2003).

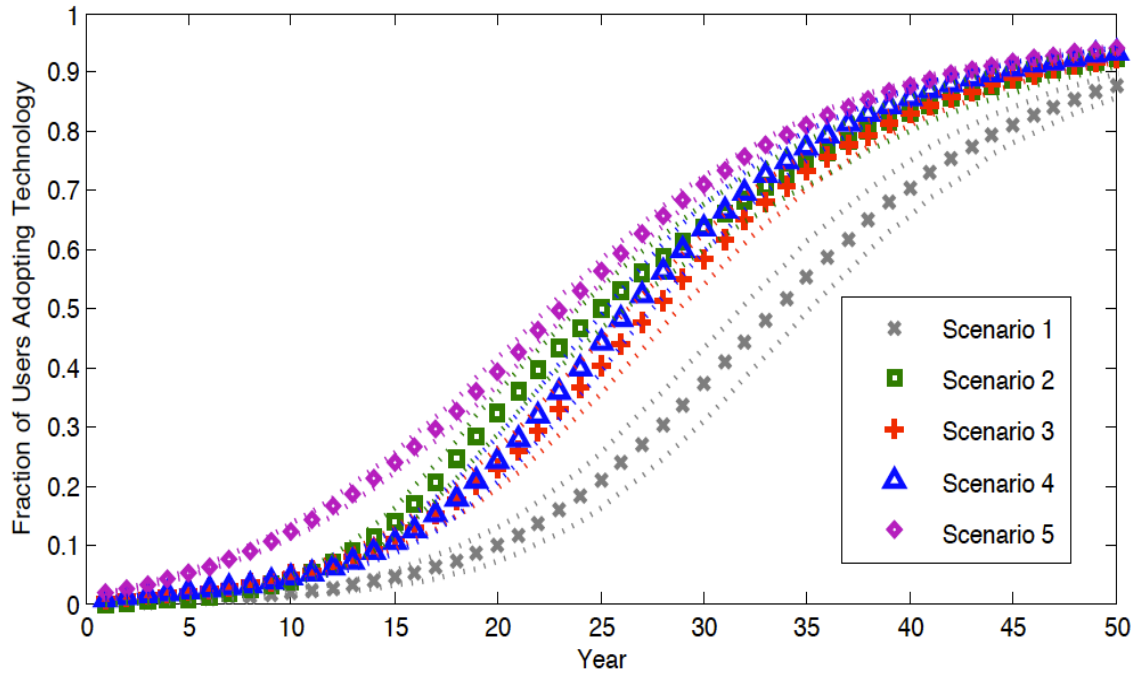


Figure 3. Comparison of the fraction of agents adopting switchgrass over time under five different policy scenarios. Dashed lines indicate one standard deviation of the results obtained by running the model 20 times.

Figures 2 and 3 describe some interesting aspects of the model demonstration. The model results suggest that all policy instruments (Scenarios 2-5) enhance the rate of switchgrass penetration relative to the baseline case (Scenario 1). As expected for Scenario 2, an increase in profitability significantly increases switchgrass adoption in Region B (the right portion of the grid), which would be expected by the increased profitability of these farms. For Scenarios 3-5, demonstration farms which provide outreach and education are distributed through the region in three patterns: random (Scenario 3), uniformly gridded (Scenario 4), and clustered (Scenario 5). Although an identical number of switchgrass demonstration farms are included at the beginning of Scenarios 3-5, different adoption patterns result from their initial spatial orientation.

Both Scenarios 3 and 4 display increased adoption from the baseline case; however, whether the farms are uniformly or randomly distributed does not appear to have much impact on overall adoption. Scenario 5 has the same initial number of demonstration farms as Scenarios 2 and 3, but shows a significant increase in overall adoption. These results suggest that clustering higher concentrations of demonstration farms and/or educational efforts in targeted areas may have a greater impact on overall adoption than a lower concentration spread over a larger region.

The simulation results conform to general expectations of adoption patterns, and show how different policies may be implemented to influence adoption probabilities throughout the system. The results of the demonstration are merely suggestive and intended to show proof-of-concept. Intensive exploration of parameter derivations, model sensitivity, and validation are necessary to inform a robust analysis.

<heading level 2> ***Step 4: Integration of Scenario Results into LCA***

Similar to the approach described by Davis and colleagues, the LCI is calculated after each time step in the scenario model (Davis et al. 2009). The model outputs include the overall market penetration of the technology over time as well as the number and spatial orientation of agents in each attribute category that have adopted the technology. The LCA practitioner must identify the elements of the LCA that are different for each type of potential adopter. Each agent that adopted the new technology is assigned LCI information according to its adoption pathway.

To integrate the scenario model into the LCA framework, the LCA practitioner determines the LCI for each adopter division and determines the overall LCI results depending on the mix of adopters identified by the scenario model. For systems with a major geographic consideration, such as bioenergy, solar field development, or urban metabolic studies, GIS can be used to better understand the model and spatial distribution of technology adoption and region-specific environmental impacts such as smog formation, acidification, and eutrophication.

LCI data must be collected for each land conversion scenario that corresponds to each adopter division. In the switchgrass case, the inventory is expected to be different

1 for actively managed agriculture and marginal land. After each time step, LCI data are
2 added for the agents who have adopted switchgrass. Relevant inventory data include net
3 GHG emissions from land use change and shifts in agricultural practices, nutrient and
4 pesticide runoff, erosion, and other major emissions associated with agriculture. The net
5 change in the emissions inventory is obtained by subtracting the switchgrass conversion
6 maps from the baseline map. This information can be used to determine whether
7 geographic and temporal considerations have a significant effect on switchgrass-to-
8 energy LCA results. It can also suggest improvement or necessary policy drivers to
9 improve system performance.

10 Model results of the switchgrass system can be used to inform a number of
11 interesting analyses. For the switchgrass example, the grid in Figure 2 can be divided
12 into two divisions. At the initial state, the top half of the region is planted entirely in
13 cotton and the bottom half of the region is entirely land set aside for Conservation
14 Reserve Program (CRP). Because the attribute categories are randomly distributed and
15 there are no significant differences in the adoption patterns of the top and bottom halves
16 of the geographic region for any of the scenarios, half of the switchgrass adopters would
17 have previously been cotton farmers and half would have been enrolled in the CRP. The
18 aggregate LCA results would be evenly split between cotton-to-switchgrass adoption
19 pathway and the CRP-to-switchgrass pathway. It is not advisable to simply average the
20 results of the two adoption pathways, which reduces the resolution of the LCA
21 information. Instead, this information should remain distinct to show the relative LCA
22 for different adoption pathways and the anticipated contribution of each pathway to
23 overall switchgrass adoption. In reality, the relationship between adopter divisions and
24 attribute categories will not be random and may show a preference for one type of
25 adopter division to predominate the LCA.

26 In addition to the biogeochemical differences of previous land patterns, adopters
27 in nitrogen-limited regions have different eutrophication impacts than those in
28 phosphorus-limited zones. Iterative LCA results can be used to determine policy
29 implications on adoption probabilities of landowners and the subsequent LCA results.
30 Additionally, the spatial information and extent of adoption may also change LCA

1 results. Figure 2 suggests how different policies may impact clustering of switchgrass
2 farms. The extent of potential adoption within a region may dictate the logistics and
3 viability of a switchgrass-to-energy industry. For example, greater clustering behavior is
4 expected to reduce transportation distances and may provide better economies of scale
5 than a less clustered adoption pattern.

6 <heading level 2> *Parameter Derivation and Validation*

7 One of the major difficulties in the proposed modeling effort is calculating realistic
8 estimates for each of the possible attribute categories, $p(S|a_i)$. The proposed method
9 relies on probability calculations that may require uncertain or missing information. The
10 likelihood $p(X|S)$ and normalizing probability $p(X)$ are needed for each attribute
11 category, as well as the initial prior probability of planting switchgrass $p(S)$. These
12 probabilities may be inferred from literature, obtained through survey methods, or
13 elicited from expert opinion. One possible method using the switchgrass example is
14 given in the Supporting Information.

15 The likelihood terms $p(X|S)$ can be obtained from decision-making patterns or
16 from consultations with experts. Research on agricultural decision patterns is available,
17 and the body of knowledge is growing (Hipple & Duffy 2002, Jensen et al. 2007,
18 Ridgeley & Bush 1992, Rogers 1995, Saltiel et al. 1994, Thomas et al. 1990, Vander Mey
19 2004). In addition, once the prior probabilities and likelihood information are obtained,
20 the probability of each of the 27 classes of decision makers can be determined.

21 One of the major difficulties with this model is determining an initial prior
22 probability, $p(S)$, for a system that has not developed. The value of $p(S)$ dictates the rate
23 of overall adoption within the system, and scenario results are sensitive to this parameter.
24 $p(S)$ will generally be a small, highly uncertain number given a new and unfamiliar
25 technology. The method for determining this value will be different for every situation;
26 however, historical trends can often be used to generate a reasonable estimate. Therefore,
27 the differences in scenarios relative to the reference case may be more meaningful than
28 the actual adoption curves, given the uncertainty surrounding $p(S)$ for emerging systems.

As with any model, the described adoption framework must be subjected to rigorous sensitivity analysis and validation. Adoption curves can be highly sensitive to behavior attributes (Rogers 2003). For this reason, the framework can be used to understand general trends, but should not be used as a predictive tool. To test model validity, calibration and validation with data sets from previous technology diffusion is possible. Diffusion patterns for a variety of technologies have been published in literature (Deffuant et al. 2005, Morris & Venkatesh 2006). For data specific to the switchgrass case study, technology adoption and innovation diffusion has also been studied with respect to agricultural populations (Sundling & Zilberman 2001, Just & Zilberman 1983). The prevalence and diffusion of new crops or agricultural practices within a region can give reasonable basis for comparison.

<heading level 2> *Comparison to Alternate Modeling Approaches*

Although Bayesian probabilities are proposed in this framework, there are other modeling techniques that could be used. For example, decision making by an individual agent could be represented using an absorbing, non-homogeneous Markov chain (Ibe, 2009). This type of model is more complex than a traditional homogenous Markov chain as state transition probabilities must adapt throughout the simulation in response to changes in the agent's adopter class. Applying a Markov type of analysis would provide a powerful toolbox for analyzing the ensemble behavior of the agents. In this work, we have chosen to avoid this formalism since the described simulation is expected to be conceptually easier to understand and implement by practitioners.

In the switchgrass case study, we explicitly tied each agent to a regularly gridded land unit for conceptual simplicity. The resulting simulation illustrated in Figure 2 has the appearance of a cellular automata model (Sante et al, 2010). In practice, however, it would be reasonably straightforward to assign agents to one or more irregular land units. In addition, the decision rules in our model are not based directly on interactions between adjacent cells as is typical in cellular automata models. In our approach agent interactions are enforced through the familiarity attribute. Although we quantified the familiarity attribute using a spatial measure of distance, it could also be quantified using alternative metrics, such as social distance. Our model is similar to the work of Kocabas

1 and Dragicevic (2006), which coupled Bayesian networks with cellular automata to
2 model land use change based on underlying attributes derived from GIS analyses. The
3 approach may be best classified as a hybrid model that links agents as decision making
4 entities to an underlying cellular model of the environment (Parker et al., 2003).

5 <heading level 1> **Conclusions**

6 This paper presents a method to determine the effect of system emergence on
7 LCA results. The established techniques can be used for any developing system where
8 technology adoption occurs and adoption patterns are expected to have an impact on the
9 LCA. This method can address one of the key challenges of trying to quantify the
10 environmental impacts of a non-established system, by coupling scenario modeling
11 results and LCI information. The spatial-temporal modeling adds a dynamic component
12 that also assists in the understanding of developing complex systems and the aggregate
13 effect of a technology change.

14 While the framework can be useful, there are also potential drawbacks. Data
15 availability and uncertainty will always be problematic. It is therefore recommended that
16 this framework be used to understand the system dynamics and implications of certain
17 development patterns rather than as an actual predictive tool.

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Figure Captions

Figure 1. The framework for integrating the stochastic model into LCA. Each agent is classified into an attribute category a_i . Each attribute category has a probability of adoption, $p(S|a_i)$. Life cycle inventory information is compiled according to the proportion of adopters having different baseline characteristics.

Figure 2. Schematic showing a spatial representation of model progression of switchgrass adoption over time for five different scenarios (rows 1-5) at $t=5, 10, 15$, and 20 years (columns 1-4). Black dots indicate a landowner that has adopted switchgrass.

Figure 3. Comparison of the fraction of agents adopting switchgrass over time under five different policy scenarios. Dashed lines indicate one standard deviation of the results obtained by running the model 20 times.

Box Captions

Box 1. Basic primer on Bayes Theorem

Box 2. Example calculation of adoption probabilities

Table Captions

Table 1. Model scenario descriptions