COMPLEMENTING LIFE CYCLE ASSESSMENT BY INTEGRATED HYBRID MODELING AND SIMULATION

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ABSTRACT
This paper presents a new complementary life cycle assessment (LCA) approach to address several limitations of the standard LCA methodology thus enhancing the functionalities of environmental impact analysis. The research demonstrates that the hybrid modeling and simulation method can address some of the limitations of the standard LCA, which were results of the assumption that parameters and relationships are constant regardless of local uniqueness. Also, the method is demonstrated to have a potential to address social and economic aspects as well. The hybrid simulation model was developed as a proof-of-concept system, which was validated using a case study of bottled water and alternative drink products.

Keywords: Sustainability, Life Cycle Assessment (LCA), Agent-Based Modeling, System Dynamics, Discrete-Event Simulation

1. INTRODUCTION
Sustainability issues are being addressed by a variety of different activities ranging from creating environmental-friendly products to changing habits to reduce waste. While such initiatives deserve commendations, there is a danger of narrowly focusing on local optimization thus unintentionally worsening the whole situation unless a holistic systems thinking guides those executions. One of the tools available to assess overall environmental impacts throughout a product's entire life is life cycle assessment (LCA). LCA is the "compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle" (ISO 14040, 1997). In a LCA study, many aspects throughout a product's lifecycle can be considered ranging from production, transportation, distribution, usage and ultimately to the end-of-life activities.

However, the standard LCA method has a number of limitations and some of these problems are critical (Reap et al., 2008). For example, the LCA method takes a static viewpoint that its parameters and internal relations among entities remain constant. Therefore dynamics among entities cannot be addressed. Also, the social and economic impact, local environmental uniqueness, effects of dynamic environment, and temporal perspectives are not easily considered in the LCA. In other words, the standard LCA is useful as a high level tool, but not for necessarily dealing with dynamics, uncertainties and broader perspectives.

This research demonstrates that a hybrid simulation model can address these limitations of the standard LCA approach. All the steps in LCA, goal and scope definition, inventory analysis, and impact assessment, including interpretation are considered in our research. However, the focus is placed on the third step of the standard LCA, that is, impact assessment. A hybrid simulation model combining agent-based modeling, system dynamics and discrete-event simulation methods was developed as a proof-of-concept system. The validity of the developed approach was done on comparing bottled water alternatives such as tap water and vitamin water along with different bottle options. The case study drew necessary data from the Nestlé report (Nestlé Waters North America, 2010).

The paper is organized as follows. First, the integrated hybrid modeling and simulation method developed for this research is presented. Drinking water and beverages is chosen to illustrate how the framework is developed and modeling is carried out. Impact analysis based on the simulation results is explained to show the value and potential of the new complementary LCA approach. Conclusion and future work is provided at the end.

2. INTEGRATED HYBRID MODELING AND SIMULATION METHOD
The hybrid model integrates three commonly used modeling and simulation methods: i) Discrete Event Modeling and Simulation (DEMS), ii) System Dynamics (SDMS), and iii) Agent-based Modeling and Simulation (ABMS). These are integrated to simulate the life cycle process and study the feasibility of complementing the functionalities of the standard LCA method. The integrated hybrid model combine the uniqueness and advantages of each of the above three methods into a single model while taking their differences into consideration.

Discrete Event Modeling and Simulation (DEMS) can simulate multiple events in a time sequence (Zeigler, Kim and Praehofer, 2000). Basic elements are entities, flowcharts and resources. DEMS is a natural choice when linear processes in a complex environment is modeled and an entity's action is triggered by other entities or at a certain time.

System Dynamics Modeling and Simulation (SDMS) is a methodology used to model and simulate a system from a higher system-level viewpoint (Forrester, 1968; Doebelin, 1998; Sterman, 2001). Stocks, flows and unique feedback loops are their basic elements. Aggregates are linked through aggregated mechanisms implemented as flows in SDMS. Feedback loops link each module of the system with defined relations and influence. The state of the whole system could be observed from various stocks at any given time.

Agent-based modeling and simulation (ABMS) is a methodology to model and simulate individual actions and interactions of agents in a complex adaptive system, focusing on their effects on the system as a whole (North and Macal, 2007). They are constructed in the form of active objects, individual behavior rules, and direct or indirect interaction within a dynamic environment.

The most promising part of the integrated modeling approach is its flexibility that can handle dynamic and evolving requirements of a system. SDMS can deal with aggregates at the highest abstraction level while DEMS can be used at middle level of abstraction and possible at lower level as well. ABMS can be used across all levels of abstraction. In our research, we utilized the flexibility of the integrated hybrid modeling and simulation and developed a proof-of-concept system that can complement the standard LCA method.

3. LIFECYCLE ASSESSMENT OF DRINKING WATER AND BEVERAGES

Tap water is still one of the major drinking sources in daily life. However, the bottled water market in developed countries such as United States and Japan has grown rapidly. For health, quality and convenience reasons, bottled water has become a popular choice in drinking water and beverage market. The rise in popularity of bottled water has created a burden on the sustainability (Gleick, 2010), however. For example, bottled water produces wastes during its production, transportation, distribution, refrigeration and recycling. So the basic questions to address by a LCA study are:

i) which one of the available options (e.g. tap water, bottled water, and other drinking alternatives) is the most sustainable?
ii) will consumers' choice make a difference?

Normally, a LCA study consists of three distinct steps with associated interpretation of results. The three steps are: i) goal and scope definition, ii) inventory analysis, and iii) assessment of impacts associated with these inputs and outputs.

3.1 Goal and Scope

The goal of our study is to measure the environmental impacts of beverage consumption habits under different scenarios. In this study, the critical environmental issues and responsibilities were identified along the entire life cycle chain of five specific drinking alternatives:

1. Tap water in glass bottle,
2. Tap water in reusable aluminum bottle,
3. Ecoshape bottled water,
4. Sport drink, and
5. Vitamin water.

Consumer behavior is also taken into consideration. Consumers are allowed to choose freely from drinking alternatives and switch among them over time to reflect the trend of consumers. Two particular impacts, energy consumption and global warming potential, are assessed to reveal the practicality of the new methodology.

3.2 Inventory Analysis

a) System Boundary

The whole lifecycle of drinking alternatives will be covered. For the sport drink as an example, its lifecycle consists of beverage production, package production, transportation, distribution, refrigeration to recycling or landfilling disposal. The boundary of the system and stages are shown in Figure 1. There are five stages in the sub-model of sport drink.

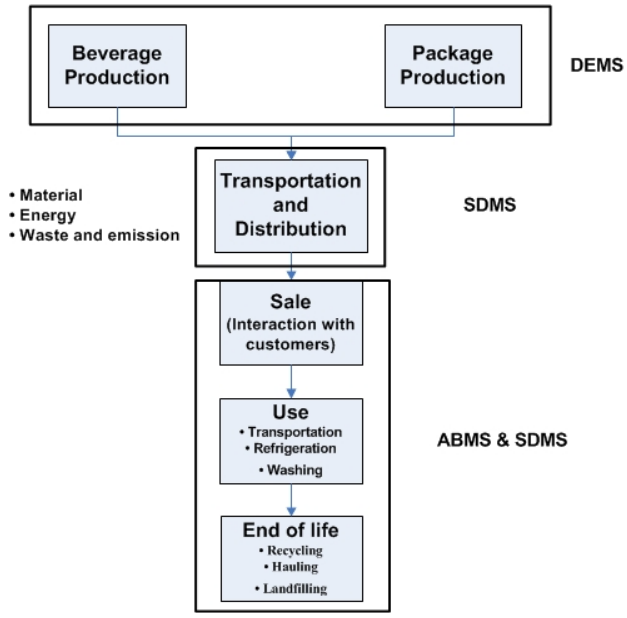


Figure 1: The boundary of the system and the stages of sport drink systems

b) Functional Unit and Emission Data

A reasonable water/beverage consumption amount is chosen as 3 liters (L) per day per person. This is equivalent to 6 bottled water volumes or vitamin water bottles. Data for material/energy consumption, water usage, waste generation, greenhouse gases emissions, distribution selection, quantitative relations between entities and parameters are collected from the Nestlé study paper (Nestlé Waters North America, 2010), GaBi databases (LBP, 2009) and published LCA papers (Azoulay et al., 2001; Keoleian et al., 2009).

c) Assumptions

In order to effectively reflect and compare the results of each product in different scenarios, the most commonly used and important two impact categories are chosen:

i) Energy that is the amount of energy used during each phase of the life cycle and Global Warming Potential (GWP) for each phase of the life cycle (Pasqualino, Meneses & Castells, 2011).

ii) Global-warming potential (GWP) is a relative measure of how much heat a greenhouse gas traps in the atmosphere. It compares the amount of heat trapped by a certain mass of the gas in question to the amount of heat trapped by a similar mass of carbon dioxide. GWP is expressed as a factor of carbon dioxide (the GWP numbers are standardized to 1).

Additional assumptions were made to simplify the model constraints and set a reference standard.

4. MODELING AND SIMULATION

System dynamics is used to model the workflow and calculate energy consumption and GWP. Since the overall process is a continuous procedure in straightforward workflow that involves plenty of feedbacks, such as material flow and energy usage, system dynamics is a natural choice. It is best suited to analyze a system with dynamic stocks, flows and feedbacks. However, the detail work processing procedure and the connection linking consumer behaviors with actions are modeled by discrete-event and agent-based methods.

4.1 Scenarios

Scenario 1 is the "reference scenario". This scenario represents the base pattern of beverage consumption in New York State assuming that only the five kinds of beverages are available. All beverages are assumed to be refrigerated for 2.4 days on average, except tap water, which is not refrigerated. The glass used for tap water and the reusable bottles are washed in a dishwasher.

Scenario 2 is similar to the reference scenario, but during the winter no beverage is assumed to be refrigerated by the consumer.

Scenario 3: In this scenario, tap water is somehow unavailable during this period, such as pollution or disaster. "tap water in glass bottle" and "tap water in reusable aluminum bottle" are then replaced by "ecoshape bottled water". All drinks are refrigerated.

Scenario 4: Under this scenario, bottled water is banned.

Scenario 5: Same as the reference scenario, but refrigeration conditions are different. It is assumed that refrigeration takes place for 7.2 days instead of 2.4, in a 20-year-old refrigerator that consumes three times more energy. Furthermore, it is assumed that the beverage occupies about 1/10 of its refrigerator content.

Scenario 6: Same as the reference scenario, but glasses and bottles are washed by hand with cold water.

4.2 Framework and Modeling

a) Overall hybrid modeling framework

The model is developed in two main parts: i) modeling the life cycle of each beverage and ii) modeling the behavior of each consumer of the population. The life cycles of the five beverages are first modeled in SDMS, followed by the consumer behavior modeled in ABMS and DEMS. The integrated model is then established in order to compare the environmental impacts of beverage consumption under the different scenarios.

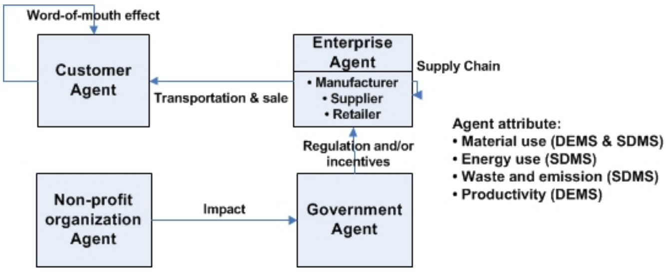


Figure 2: Hybrid model structure

b) SDMS part

Bottles, glasses and cardboard used to produce bottled water can be recycled into new containers as a feedback system illustrates in Figure 3. This increases the production rates of beverages and containers. Four kinds of raw materials are needed to manufacture bottles and their packaging: packaging cardboard, PPlid, PET Resin, and Pallet. The production rate of each beverage and each container is based on average consumer consumption (6 servings a day for one consumer) and on average losses (some bottles and glasses are stolen or damaged in the supermarkets or during manufacturing and transportation).

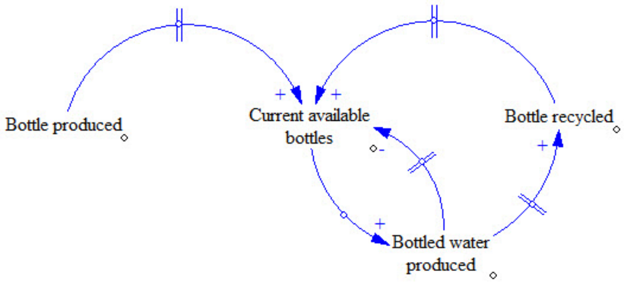


Figure 3: Bottled water production feedbacks in system dynamics

After the production stage, the beverages are transported to the marketplace such as a supermarket. There, bottles beverages are refrigerated before being sold to the consumer. After people drink the beverages, there are 3 ways to dispose all materials: i) landfilling, ii) waste-to-energy, iii) or recycling. The recycle rates depend on the container used.

For the tap water as well as the bottled beverages (ecoshape bottle, sport drink and vitamin water), the SDMS diagram is composed of two independent SDMS diagrams: one for the tap water and the other for the containers. Tap water is processed and generated at a municipal water plant, then distributed through pipes to the consumers. The tap water consumption is determined by adding: i) the tap water that is drunk by the consumer, ii) the tap water that is used for dishwashing and, iii) the losses during the production and distribution processes. The production rate of tap water is determined to meet customer's demand. On the other hand, glass bottles are produced from raw materials and reusable aluminum bottles are from recycled materials. Their production rates are chosen with respect to the consumer demand. They are then distributed to the marketplace, bought by consumers, used and then discarded.

c) ABMS and DEMS part

Starting with potential users, when they go to the supermarket to shop for their favorite products, and every purchase transaction is based on the availability of their favorite products. Customers will recycle used products and buy new products after a certain period, such as the product's lifecycle length or any replenishing time. DEMS is embedded in the statechart of agent behavior, where the state of agent will change to another state when time elapse or by certain rate depended on variables. The state such as purchase or discard may happen even by triggering certain requirements, such as word-of-mouth effect, favorite product is unavailable, etc. The sequence of discrete events is usually one-way and follows time sequence, while two-way conversion is comprised of two one-way discrete events.

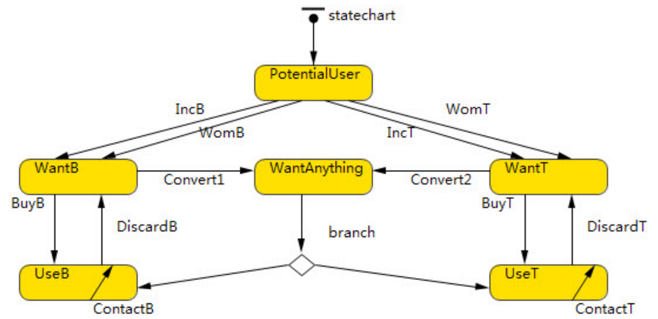


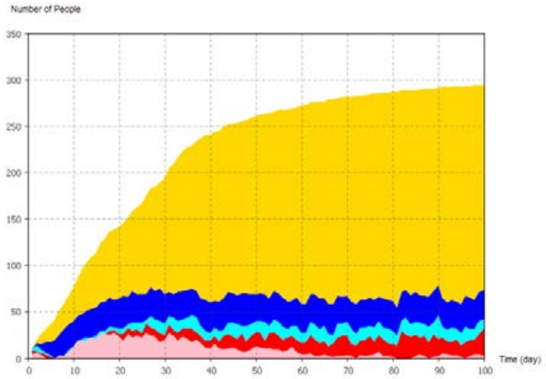
Figure 4: State chart of customer behaviors on two competing alternative products

4.3 Results and Validation

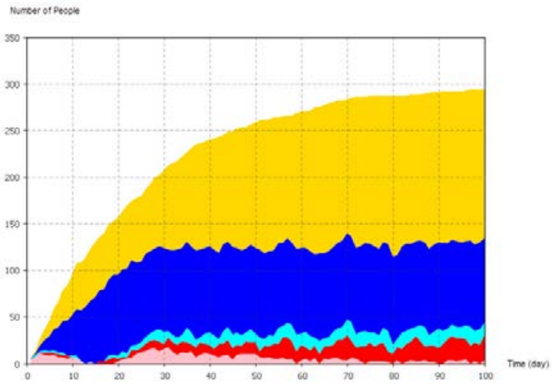
a) Observations

Three most important factors affecting the simulation outcomes are supply chain capability, customer involvement impact and market specialty. In the model, environment-sensitive behaviors were considered. There are a certain adjustable percentage of customers who prefer energy-efficient products over alternative choices. The energy efficiency calculation is based on the ratio of each product's energy consumption over total consumption amount, which leads some people to make a conversion when a more energy-efficient product becomes available.

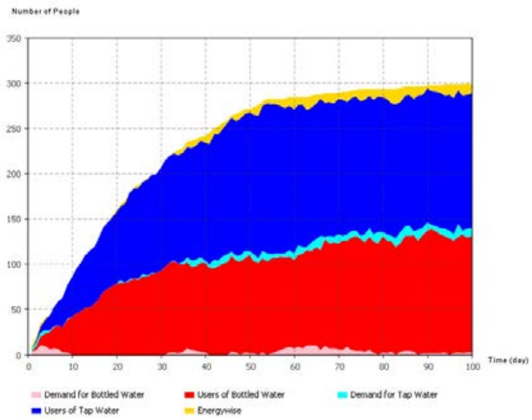
First, the characteristic of supply chain capability is studied. Figure 5 shows the market share of each product in different colors. It compares three scenarios, the replenishing period time changes from the shortest in scenario (i) to the longest in scenario (iii) while keeping all other parameters constant. X-axis represents the timeline of simulation. Y-axis represents the number of customers. The total numbers of customers reaches 300,000, which is the asymptotic value of total number of customers who would make the purchase. Customers waiting replenishment are represented in yellow color. They are potential customers in the market but without a decision to purchase any product. The yellow zone shrinks from left to right when the replenishing time increases, indicating the supply chain is capable of meeting the customer demand in longer replenishment time scenarios. The supply chain, especially manufacturer is a bottleneck in terms of production and transportation when they need to meet customers' demands in faster pacing situations. It is interesting to note that tap water in blue and bottled water in red become favorite choices at steady state situations, while sport drink in cyan and vitamin drink in pink come to represent smaller segments of the market.



(i)



(ii)



(iii)

Figure 5: Comparison of market share in three different replenishment time scenarios: (i) the shortest time, (ii) the average time, (iii) the longest time

b) Verification and Validation

The results obtained from our hybrid model for the three bottled beverages (ecoshape, sport and vitamin) are reasonably close to those reported in the Nestle report (Nestlé Waters North America, 2010), for both Energy and GWP.
Table 1 lists the LCA problems addressed in this paper and corresponding verification and validation methods adopted to caliber the hybrid model and make sure it reflects the characteristics of the competitive bottled water market.

Table 1: Verification and Validation methods

Traditional LCA problems addressed in the paper	**Modeling method**	**Result verification and validation**
Social and economic impacts	ABMS	Customer behaviors, regulation or incentives and competitive Market
Alternative scenario considerations	DEMS, SDMS & ABMS	Different local uniqueness, season and preference, customer behaviors
Local environmental uniqueness	DEMS & ABMS	Different input represents various local environments
Dynamics of the environment	SDMS & ABMS	Customer-driven market and agents make decisions on feedback
Time horizons	DEMS, SDMS & ABMS	The trend alters according to different time span
Uncertainty in the decision process	DEMS, SDMS & ABMS	Most parameters and relations have certain uncertainty range with robust analysis

c) Summary

Bottled water is regarded as a major pollution source given its energy consumption and after-use disposal method such as landfill. It was found that bottled water, which is a very common choice for users in the USA, is the third best choice overall after tap water with glass and reusable aluminum bottle. It is the second best choice as a beverage source for the environment. Water production takes a large portion of energy consumption in bottled water production (larger than distribution and transportation consumption), while other soft drinks production take extra steps to produce beverage or packaging and recycle steps, which makes them less energy-efficient or environmentally friendly if the recycling rate is the same for all products except tap water.

Word-of-mouth effect is non-negligible. However, initial customer inclination is not sensitive according to market share and energy usage, since the conversion from one product to another along with customer's influence is complementarily strong. It was also found that having a regional supply chain helps national or international manufacturers to bring down cost and environmental impact and also attract more loyal customers.

5. CONCLUSION

Usually, bottled water is not thought of as an environmentally friendly choice, the results from this study affirms it, given that energy consumption and GWP of ecoshape bottled water are 32 times and 10 times larger, respectively, than those of tap water in glass bottle. However, it is also indicated that although falling far behind the best two choices, bottled water is a good (third-best) choice. This is way better than sports drink and vitamin water both in energy efficiency and GWP emission.

Energy and greenhouse gas emission are found to be positively correlated. So energy usage can be used as a gauge to measure and evaluate efficiency and environment friendliness. The results of the hybrid DEMS-SDMS-ABMS model are good and promising, which not only matches published reports but also extend further to incorporate customer's behaviors and market responses.

For future work, other factors such as customer behavior comparison, reusable product introduction and model validation can be included to provide more comprehensive results. Washing glasses and bottles plays an important role in the life cycles, as water needs to be heated whether dishwashing takes place in a dishwasher or in a sink. It is interesting to compare the reference scenario with this one in which the dishwashing water is not heated. Customer behavior comparison is another potential subject of study. Some customers may choose the least expensive products only, while others prefer to follow the current fashion from time to time. Such customer behaviors are interesting to recognize and compare.

When more accurate data become available, more quantitative analysis beyond Design-Of-Experiment can be implemented. Products such as sports drinks, coffee, and tea can be added to study a more complete beverage market. Cost analysis could be done when pricing data is available. Parameters such as transportation distance variance were not taken into consideration. There are critical values of some parameters that exist which optimize the performance. To minimize the impact to the environment, public advertising and broadcast is effective due to the word-of-mouth effect. Government environmental and/ or production policy can impact environmental issues by limiting certain products and promoting others via incentives if they are more environmentally friendly and energy wise.

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