Life Cycle Assessment and Sustainability Analysis of Lignin Derivative Products, Materials and Technologies. Integrated Process Modeling, Scientific framework and LCA for Assessing Sustainability

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Abstract

This paper aims to develop a novel scientific model framework to assess the life cycle sustainability of lignin derived chemicals and compare the life cycle profiles of both current state-of-the-art processes and emerging lignin processes based on the value of the final products. In this work, we try to develop and implement a model to determine and to optimize the economic and environmental dimensions of sustainability and assess the sustainability of a project and possible pathway to reach a certain product. Graph theory has been established as promising way to efficiently analyze different problems like ecological assessments and supply chains. LCA can be investigated using the tools of graph theory to overcome the complexity of traditional Matrix-based analysis. The traditional greedy Dijkstra's algorithm will be modified and combined to dynamic programming approach to conduct a trade of between shortest path and longest path problem. The resulting path takes both economic and environmental performance into account in product/process design decision making.

Keywords

LCA, Lignin derivatives, Dijkstra's algorithm, Dynamic Programming

Introduction

Life Cycle Assessment (LCA) is a well-known and widely used approach to assessing the potential environmental impacts and resources used throughout a product's life cycle, including raw material acquisition, production, distribution, use, and end-of-life phases [1]. Currently, life cycle thinking plays a significant role in environmental policy making. Renowned institutions such as the World Resource Institute (WRI), have adopted life cycle thinking. As a result, the stakeholders are controlled to reduce the environmental impacts associated with their products. The LCA provides the quantitative and scientific bases for all the involved activities. Economic, environmental and social dimensions of sustainability need to be addressed in assessing the sustainability of a project, product, etc. Also, a scientifically based Sustainability Analysis necessarily involves value judgments, assumptions, scenarios and uncertainties. Generally, LCA consists of four steps including "Goal and scope", "Life cycle inventory", "Life cycle impact assessment" and "Interpretation" [1]. The LCA is typically restricted to environmental aspects, while sustainable assessment, SA, is a "broader" concept, which covers more dimensions or aspects than LCA. So, to "broaden" the scope of the LCA the social and economic dimensions should be added to the environmental LCA. Klöpffer (2008) suggested a conceptual formula for conducting a life cycle sustainability assessment (LCSA) which includes an LCA, a life cycle costing (LCC) and a social life cycle analysis (SLCA), done in a consecutive way.

$$LCSA = LCA + LCC + SLCA$$

The aim of this paper is to develop a novel scientific model framework to evaluate the life cycle sustainability of lignin derived chemicals and to compare the life cycle profiles of both state-of-the-art and emerging lignin processes based on the value of the final products [1], [2],

Process Description and System Modeling

In fiscal year 2013, SD EPSCoR and North Dakota EPSCoR1 received an RII award to conduct research on converting "lignin" - a constituent of the cell walls of almost all dry land plant cell walls- to high value chemicals that could replace petroleum-based chemicals. The specific

[1] http://www.sdreadytowork.com/News-Media/Press-Releases/SD-EPSCoR-Awarded-$20-Million-Grant.aspx

experimental process streams demonstrated the feasibility of applying high temperature hydro-treatment for production of synthetic organic polymers that already which have commercial applications. In this study, we will modify and employ different models to create a reference architecture for the life cycle assessment of probable lignin derivative products, materials, and technologies. First, technical models describe the principal causal relationships connecting the level of two economic activities. Then, physical models explain constraints and potentials of a technology system. Physical models determine whether a possible path for production of a certain product exists or not. In addition, physical models provide the conversion ratios and input-output data –mass and energy balances- for the system. The physical model inputs include proximate analysis of received lignin, multi-step reaction kinetics of lignin degradation (based on the results of the DakotaBioCon lignin processes), and results of the dynamic and economic simulation of the processes for energy consumption purposes. Chemicals emitted to the environment, will enter the environmental domain and are considered in environmental models. Furthermore, the data and costs regarding the environmental impacts can be provided from different LCA software packages. The life cycle assessment modeling software packages *i.e.* SimaPro v.8.0, can be employed to develop and to analyze the proposed model. The inventory data for biomass handling, including all activities, can be collected from reports, surveys and the literature. The output of the LCA software for certain paths are considered as the environmental cost, which will be discussed later in this study. For now, we are using generic data for the environmental impacts and the kinetics of the real pathways - sample data- to check and to evaluate the model. The socio-cultural, institutional and political considerations are also involved. For example, a technology may not be accepted or only slowly accepted, (like nuclear technologies), which are considered in cultural, institutional and political models [3]–[5] .In this study, for model development and optimization, the Soci-cultural models and inputs are excluded because of two reasons: first, for simplification purposes; as developing and optimization of a model with three different variables would be more complicated; secondly, still no solid agreements exist on the metrics of the social aspects.

The proposed model, presented in figure 1, is a generic single input - multiple output problem. The intermediate chemicals (Eugenol, Guiacol, Vanillin, etc.) are possible lignin derivative chemicals obtaining through different thermal treatments of the lignin. The “treatments” represent different thermal conditions (different temperature, pressure, catalyst etc.) of the source material- in this proposal the lignin -and K_1, K_2 and K_3 represents the yields of conversions which can be defined by the user. Again, from a certain hydro-treated state, we can produce different intermediate chemicals through different reaction pathways. These pathways would have their different conversion yields which is defined as $K_{i,j}$ in the model. Likewise, we can continue the same procedure until we reach the final products. In every single step, different K's are defined based on the conversion factor which will be used in the model. *K* values show the yield factors based on 100% conversion of the initiator and can be zero when there is no conversion. Apart from the conversion factors, the environmental emissions should be defined. The output of LCA software packages can be employed as the environmental factor for each path. Therefore, the user can check the environmental and economic cost of a possible pathway for different chemicals with different yields.

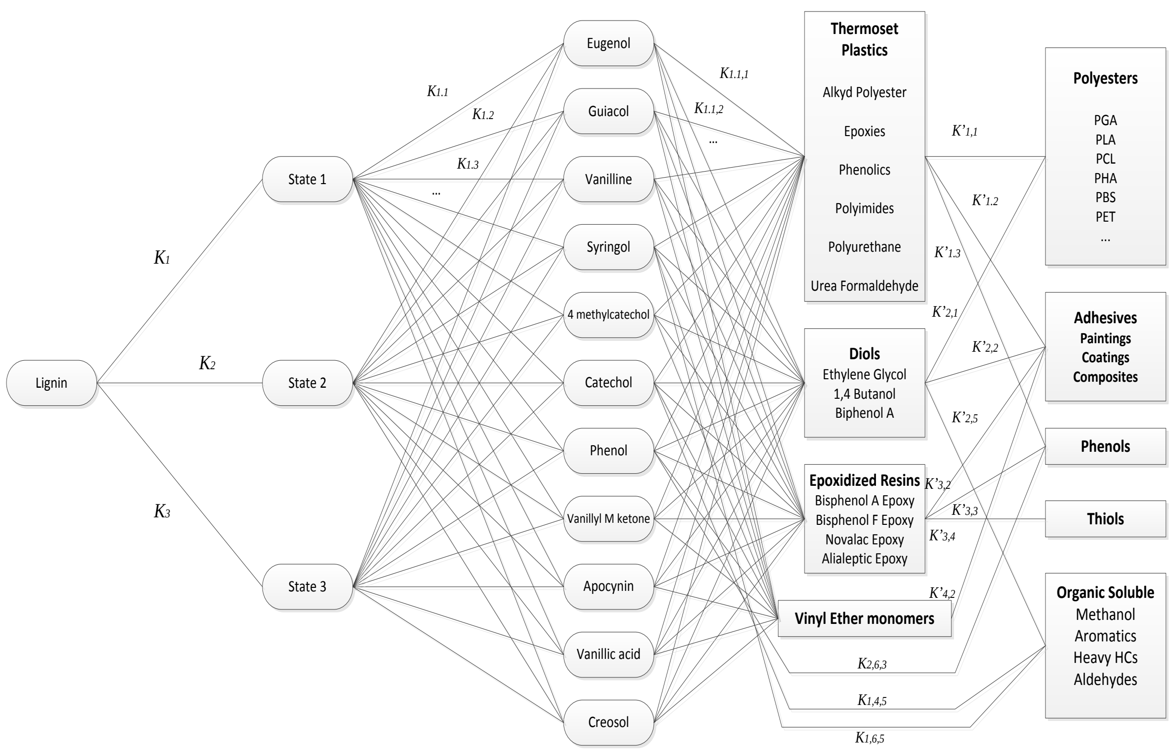

Figure 1, Pathways for Chemicals derived from Lignin, Multi objective optimization

If an option is not feasible (which in lignin project means that production of that certain chemical is not feasible in that pathway) with respect to the first priority objective function, then it does not proceed further. When the improvement is not possible, then the next prioritized option will be selected. The proposed optimization approach will allow the assessor to consider all options, select the most beneficial option, and identify possible areas for improvement even for future progresses [6].

Multi-objective Optimization for Decision Making

Life Cycle Analysis can be investigated using the tools of *graph theory* to overcome the complexity of traditional Matrix-based analysis. Since the graph is derived from a technical and physical model of system, it would be an acyclic graph (graph having no graph cycles) with intermediate and final products in different pathways as nodes and edges connecting products based on their economic and environment cost. Although the whole problem is dealing with a single source (lignin) - multiple product condition, the equivalent graph is a single source-single destination depending on the final product under analysis. By manipulating the lignin hydrotreatment conditions and use of different catalysts in different operational conditions, we can engineer the pathways to a final product.

Thus, in this framework different objective functions and optimization should be carried out in order to select the optimum pathway. Starting from lignin, there would be several possible pathways to reach a target chemical as a final product. In order to design the best pathway to reach the target product, e.g. a polyester, we have to change the decision problem to the optimization problem. A modified Dijkstra's algorithm along with dynamic programming is developed to make a trade of between maximizing economic benefit and minimizing environment cost.

Environmental Analysis

Finding proper design to minimize the environmental effects in aforementioned model is equivalent to shortest-path problem in graph theory.

In a shortest-paths problem, we are given a weighted, directed graph $G(V,E)$, with weight function $w: E \rightarrow R$ mapping edges to real-valued weights. The weight $w(p)$ of path $p = \langle v_0, v_1, ..., v_k \rangle$ is the sum of the weights of its constituent edges:

$$w(p) = \sum_{i=1}^{k} w(v_{i-1}, v_i)$$

The shortest path weight $\delta(u,v)$ from u to v is defined by $\min\{w(p): u \xrightarrow{p} v\}$, and the shortest path from vertex u to vertex v is then defined as any path p with weight $w(p)=\delta(u,v)$ [7].

Shortest-paths algorithms typically rely on the property that a shortest path between two vertices contains other shortest paths within it. Dijkstra's algorithm is a well-known greedy strategy to solve the single-source shortest paths for a given graph $G(V,E)$ with nonnegative edge weights. The computational cost of this algorithm is $O(|V|\log|V|+|E|)$.

Definition of Dijkstra's Algorithm

1. To find the shortest path between points, the weight or length of a path is calculated as the sum of the weights of the edges in the path.
2. A path is a shortest path is there is no path from x to y with lower weight.
3. Dijkstra's algorithm finds the shortest path from x to y in order of increasing distance from x. That is, it chooses the first minimum edge, stores this value and adds the next minimum value from the next edge it selects.
4. It starts out at one vertex and branches out by selecting certain edges that lead to new vertices.
5. It is similar to the minimum spanning tree algorithm, in that it is "greedy", always choosing the closest edge in hopes of an optimal solution.

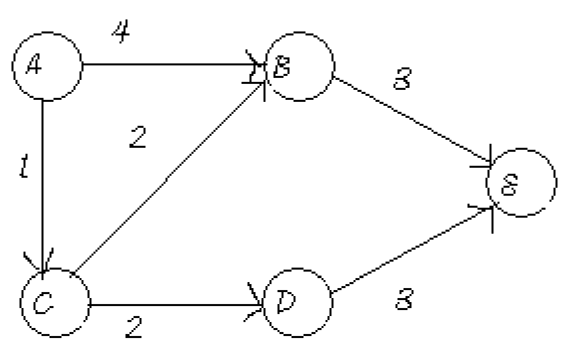

Figure 2, Example of Dijkstra's algorithm

The following pseudo-code of the Dijkstra's algorithm. The algorithm illustrates Best-First-Breadth-First-Search.

```
Procedure Dijsktra (V: set of vertices 1... n {Vertex 1 is the source}
                    Adj[1…n] of adjacency lists; EdgeCost(u,
                    w): edge – cost functions;)
Var: sDist[1…n] of path costs from source (vertex 1); {sDist[j] will be equal tothelengthofthe shortestpathtoj}

Begin:
Initialize

{Create a virtual set Frontier to store i where sDist[i] is already fully solved}

    Create empty Priority Queue New Frontier; sDist[1]←0;
    {The distance to the source is zero}

    forall vertices w in V – { 1 } do {noedgeshavebeenexploredyet}

        sDist[w]←∞

    end for;

    Fill New Frontier with vertices w in V organized by priorities sDist[w];
endInitialize;

repeat

v←DeleteMin { New Frontier } ; {v is the new closest; sDist[v] is already correct}

forall of the neighbors w in Adj[v] do

    ifsDist[w]>sDist[v]+EdgeCost(v,w)then
        sDist[w]←sDist[v] +EdgeCost(v,w)
            update w in New Frontier {withnewprioritysDist[w]}

    endif
endfor

until New Frontier isempty

endDijkstra;
```

Algorithm 1. Pseudo Code of Dijkstra's Algorithm [6], [7]

Economic Analysis (LCC)

Despite environmental analysis, economical analysis tries to find pathway with maximum profit, which is similar to longest-path problem in graph theory.

The longest path problem is finding a simple path between two nodes with maximum weights. In a weighted, directed graph $G(V,E)$, with weight function $w: E \rightarrow R$, the weight $w(p)$ of path $p = \langle v_0, v_1, ..., v_k \rangle$ is the multiplication of the weights of its constituent edges:

$$w(p) = \prod_{i=1}^{k} w(v_{i-1}, v_i)$$

The longest path weight $\gamma(u,v)$ from u to v is defined by $\max\{w(p) : u \xrightarrow{p} v\}$, and the longest path from vertex u to vertex v is then defined as any path p with weight $w(p) = \gamma(u,v)$

Finding longest path in graph is NP-complete problem which means in general, there is no known algorithm that can solve this problem in reasonable time. But it can be solved, if the graph has a special property, like being small, or being acyclic. Dynamic programming technique is effective for this type of graphs and will find the longest path in polynomial time [8], [9].

```
Initialize:
        Define length array with |V| elements of type float with default value 0
Iteration:
        For each node v in top order
            For each edge (v,w)
                if length(w) <= length(v) * + w(v,w)
                    length(w) = length(v) * + w(v,w)
Return length(w) and equivalent path
```

Algorithm 2. Dynamic programming algorithm to find longest path

Multi-objective Analysis

Due to gap between LCA and LCC analysis, a multi-objective analysis is conducted to evaluate the trade-offs between environmental and economic costs of producing products from lignin. Unlike existing approach which starts from one side and add elements of the other side, the proposed solution will optimize both problem simultaneously and find the best combined pathway.

In a multi-objective problem, we are given a directed graph $G(V,E)$, with two weight functions $w_1, w_2 : E \rightarrow R$ mapping edges to real-valued weights. The objective is to find a single path $p = \langle v_0, v_1, \ldots, v_k \rangle$ between source and destination node such that:

$$p = \langle v_0, v_1, \ldots, v_k \rangle = \arg\max \left[r_{LCC} * \left(\prod_{i=1}^{k} w_1(v_{i-1}, v_i) \right) + r_{LCA} \left(1 - \sum_{i=1}^{k} w_2(v_{i-1}, v_i) \right) \right]$$

where r_{LCA} and r_{LCC} are user defined weights for LCA and LCC analysis.

Initialize:

Define the weight of LCA and LCC

Define ratio array with $|V|$ elements of type float with default value 0

Iteration:

For each node v in top order

For each edge (v,w)

if $ratio(w) \le ratio(v) + r_{LCC} w_1(v,w) + r_{LCA}(1 - w_2(v,w))$

$ratio(w) = ratio(v) + r_{LCC} w_1(v,w) + r_{LCA}(1 - w_2(v,w))$

Return ratio(w) and equivalent path

Algorithm 3. Multi-objective algorithm

Summary and Future Work

A general method was developed to construct a LCA analysis graph for an arbitrary product with different physical model. Modified Dijkstra's algorithm along with dynamic programming was developed and implemented to assess the sustainability of a project and possible pathway to reach certain product. The generalized algorithm proposed in the present study enables all industries to model and carry out LCA analysis of their products in both economic and environmental aspect. The authors plan to add social analysis part to current model and also validate the model using real world data.

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