Integration of Machine Learning and Mathematical Programming Methods into the Biomass Feedstock Supplier Selection Process

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ABSTRACT

Recent concerns over the use of and reliance on fossil fuels have stimulated research efforts in identifying, developing, and selecting alternative energy sources. Biofuels represent a promising replacement for conventional fuels for heating and mobility applications, however, variability in the quality and availability of biomass feedstocks greatly affect the utility of biofuels due to the impact on cost and life cycle environmental performance. Thus, methods for mitigating these potential impacts are needed when selecting biomass feedstock suppliers. In the research herein, the selection of the best supplier is investigated for a biomass supply chain (BSC) network by including both qualitative and quantitative factors. Most existing supplier-selection methods consider four steps: (1) Problem formulation, where Decision-Tree Analysis is applied as a qualitative method for defining the type of biomass feedstock materials for biofuel production, (2) Criteria definition, (3) Pre-evaluation of qualified suppliers, which employs the Support Vector Machine (SVM) method, and (4) Final selection. Integration of machine learning (ML) techniques and a mathematical programming model is undertaken with this method to select the most appropriate feedstock suppliers. It is shown that integrating ML and mathematical programming methods offers a promising approach to supplementing existing supplier selection methods for biomass-to-biofuel supply chains.

1. INTRODUCTION

In recent decades, biofuel has been recognized as a potential source of energy that could have positive effects on the environment, economy, and society. Biofuel is made from organic material or biomass, grown in fields and forests [1]. A successful biofuel industry would benefit society by reducing energy and fuel costs, while reducing the imports of oil and improving energy security. Biofuel has been proposed as a replacement for conventional liquid fuels because it can reduce life cycle emissions, and their associated impacts, e.g., climate change [2]. Sharma et al. [3] provided a starting point for understanding biomass feedstocks and biofuel production and presented a review of biomass supply chain (BSC) design and modeling, specifically for mathematical programming. BSC design and modeling must account for uncertainties such as seasonality, weather, physical and chemical characteristics, distribution, and supplier agreements [4]–[6]. The BSC includes the biomass feedstock supplier, storage sites, biorefinery sites, pre-treatment facilities, and distribution [7].

Globalization and a competitive environment have lead companies to give more attention to consumer expectations, final price, product quality, and lead times. For a firm to remain competitive and achieve environmental goals, careful supply chain management is critical. Supply chains move material between the source and end-users, and consist of suppliers, manufacturers, distributors, and customers [8]. Supplier selection is a key aspect of supply chain management. Since the 1960s, several methods have been introduced by investigating different stages and characteristics of the supplier selection process. The supplier selection process has been divided into four steps: Problem formulation, criteria definition, pre-evaluation of qualified suppliers, and final selection [9]. Figure 1 indicates the steps of the supplier selection process, based on work by Aissaoui et al. [10]. In general, the two final steps of this process have been a focus of prior research [11]–[13].

In the research herein, the selection of the best supplier is investigated for a biomass supply chain (BSC) network by including both qualitative and quantitative factors by adapting the above supplier selection process. Machine learning (ML) techniques and a mathematical programming model are integrated to select the most appropriate biomass feedstock suppliers. Most decision tools for problem formulation include qualitative methods that assist

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experts and decision-makers in carefully identifying the need for a decision and the alternatives that seem to be available [10]. The first step is to identify what purchasers require of the supplier. The Kraljic Portfolio Purchasing Model is often applied to make right decisions in purchasing process [14]. Figure 2 indicates Kraljic's classification according to the potential Profit Impact and Supply Risk for each item.

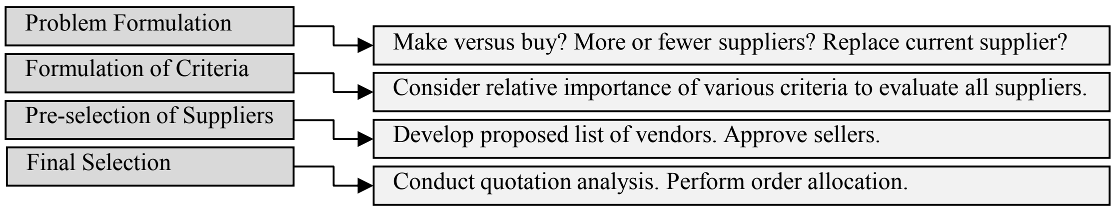

Figure 1. Decision methods in supplier selection [9].

According to Kraljic [14], Profit Impact is high when items add significant value to the company's output (product), for example items may comprise a high proportion of the final product. Supply Risk is high when items have constrained availability, for example due to scarcity, logistics challenges, or government instability. Routine items (low profit impact, low supply risk) are non-critical items produced in standard configuration. The best method of controlling these items is to optimize inventory, and there is no need to consider other attributes. Bottleneck items (low profit impact, high supply risk) are those whose supply involves various risks and problems. In this situation, contract guarantees, supplier control, and strategies to maintain high inventory levels are recommended. Leverage items (high profit impact, low supply risk) include the materials for which the buyer has maneuverability to bargain and readily available alternative products and suppliers. Strategic items (high profit impact, high supply risk) require the most attention since they are critical to ensuring high output value, but are attendant with supply constraints. The company can focus on developing long-term supply relationships, assessing risks regularly, and devising contingency plans to mitigate risk. They may choose to make the item in-house, rather than purchasing it.

2. BIOMASS FEEDSTOCK SUPPLIER SELECTION PROCESS

Biomass feedstocks are commonly classified into first (edible crops), second (lignocellulosic and other non-edible sources), and third (algal biomass) generations. The various types of biomass feedstocks can be converted into biofuels [15]. Each generation of feedstocks can be classified according to the Kraljic purchasing model depending upon their supply risks and profit impacts. The BSC includes several phases from harvesting to the arrival of biomass feedstock at the bio-refinery. An objective of this research is to develop a supplier selection process to predict BSC network cost that will account for variation in feedstock quality and variability in feedstock availability over time. The general approach is presented below.

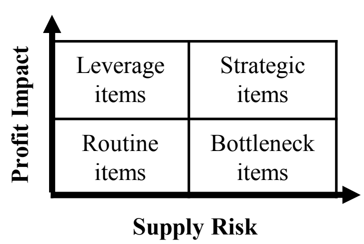

Figure 2. Kraljic's classification matrix for purchasing various items [14].

2.1. PROBLEM FORMULATION

For this step, the Decision Tree (DT) method is applied. The DT method is commonly used in machine learning and data mining. DT analysis can take categorical, binary, and numeric value input and output variables, and it can handle missing attributes and outliers well. DT analysis is also good in explaining reasoning for its prediction and therefore gives good insight about the underlying data [16]. Classification tree analysis is a DT approach usually used to illustrate the basic idea of machine learning. A classification tree approach is developed next and employed to explain the concepts as a part of the narrative. Classification tree analysis is conducted with the assistance of R.

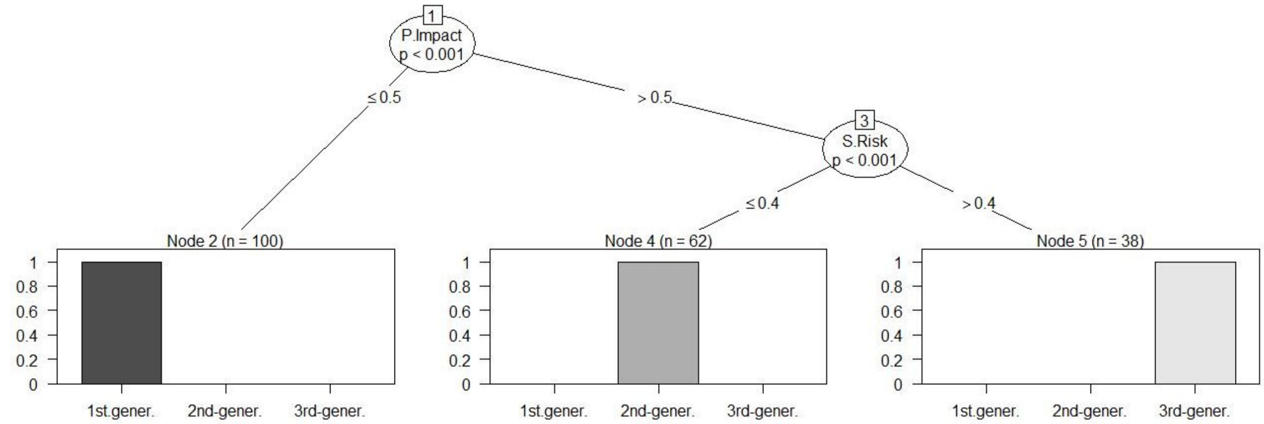

Figure 3. Classification tree for purchasing three different generations of biomass feedstock (R results).

A randomly generated dataset is used to provide profit impact and supply risk values for 200 suppliers for three different generations of biomass feedstocks. Figure 3 indicates the basic form of classification tree analysis for the three generations, which starts with all items in one group and then identifies characteristics (shown in Figure 2) that best classifies each item into one of the three generations. A random sample is chosen from the dataset, rather than stratifying by all items. Half of the data is used as a training set and the other half is the testing set. In general, DT analysis has a fairly low misclassification error rate. From the figure, for instance, it can be seen that items with supply risk > 0.4 and profit impact > 0.5 are classified as third-generation biomass feedstocks.

2.2. *Formulation of Criteria*

Supplier selection is a term used in supply chain management that refers to the process of evaluating and approving potential suppliers by several criteria. Dickson [17] identified 23 different criteria evaluated in supplier selection. Most research related to the evaluation and selection of suppliers has identified price, quality, capacity, and delivery time to be the key criteria considered in supplier selection problems. In this research, each of these factors will be considered (in section 2.3 and 2.4) due to their importance in selecting a proper biomass feedstock suppliers.

2.3. *Pre-selection of Potential Suppliers*

In this step, pre-selection is a quantitative method that evaluates and selects qualified suppliers from all suppliers. The Support Vector Machine (SVM) method is a supervised method in machine learning, and uses historical company data as inputs and outputs. SVM can provide a learning technique for pattern recognition which is reasonable in learning theory [18]. In addition, SVM is equivalent to solving a linear constrained quadratic programming problem, so that the SVM solution is always unique and globally optimal [19], [20].

A dataset of 150 suppliers provides an example for the corresponding features in each feature sample. This dataset would typically be obtained from historical data for each company, but is randomly generated for this study. The outputs for each supplier define the set of performance data for that supplier. In supply chain management, it is notably difficult to obtain this type of data, and large datasets are not readily available. Thus, the provided dataset is defined as an example for this step in order to validate the performance of supplier selection process. Table 1 shows an instance of the pre-evaluation of suppliers, including the identified key criteria. These data form the training set, which contains input and output information.

The performance of suppliers can be predicted after defining the weights for each criterion. SVM analyzes supplier data to identify any patterns that are then used for classification. SVM then uses the key criteria identified in the second step (Formulation of Criteria) as features to find the weight of each criterion. In literature, these features are called credit indexes, which are quantified from historical company data [21]. The outputs (target variables) are the final supplier credit index values that define the performance of the suppliers. The approach assumes historical data can be obtained for a given the output. It is further assumed if data is not available it can be obtained based on short-term supplier selection experiences [22]. High output scores identify suppliers that have the highest probability of being selected.

Table 1: Example of training set for supplier selection

Training data

Supplier No.	Price ($)	Constant cost ($)	Capacity	Failure rate	Tardiness rate	Output
1	7	705	66	0.07	0.9	0.89
2	5	791	61	0.11	0.6	0.73
3	10	968	69	0.08	0.8	0.69
4	9	655	76	0.05	0.8	0.8
⋮	⋮	⋮	⋮	⋮	⋮	⋮
Weight	?	?	?	?	?	

History of data

SVM finds data pattern

The training set along with the testing set are used to train and test the SVM. The provided dataset contains values for 100 suppliers as a training dataset and 50 supplier values as a test dataset. Table 2 shows SVM can find the pattern and the weights from the training information in the training phase [23]. Support vectors recognize this pattern of the data, which define the weight for each criterion.

Table 2. Identified weights from the Support Vector Machine (SVM) method (R results).

Items	Price ($)	Constant cost ($)	Capacity	Failure rate	Tardiness rate
Weight	513	569.9	481.27	56.67	56.12

The weights found in the training phase can be used to predict output (performance) in the test set (Table 3) to classify the qualified and unqualified suppliers.

Table 3. Example of test set of supplier selection.

Testing data

Supplier No.	Price ($)	Constant cost ($)	Capacity	Failure rate	Tardiness rate	Output
1	8	777	71	0.13	0.7	?
2	5	651	66	0.07	0.6	?
3	9	764	72	0.13	0.7	?
4	7	991	62	0.07	0.6	?
⋮	⋮	⋮	⋮	⋮	⋮	⋮

SVM finds performance rate

In general, the SVM learning algorithm provides us with a quantitative tool for supplier evaluation and selection. SVM has been applied for the pre-selection of potential supplier for the following reasons [22]:

- Pre-selection of potential suppliers by other methods, such as the Analytic Hierarchy Process, are an involved and prolonged task. Also, even if the company has a wealth of historical data, the training and testing tasks will take a short amount of time to identify the data pattern.
- SVM is a non-parametric and objective method, since it focuses on identifying patterns in the data.
- SVM can find a solution even if some data are missing.
- Unlike statistical methods, SVM can control large-scale problems.
- SVM is a supervised method that is more accurate than unsupervised methods, e.g., clustering analysis.

2.4. FINAL SELECTION

In the final step, after evaluating and selecting some potential suppliers via SVM methods, a mathematical model is introduced to select the supplier with the aim of minimizing the cost of purchasing biomass feedstocks, considering limitations such as capacity, quality, supply base, lead time, and other limitations when numerous sources of uncertainty exists in the BSC with respect to quality and lead time such as weather uncertainty, low bulk density of biomass feedstocks, and suppliers contracts and government policies [3]. The mentioned criteria (in step 2.2) have been used for selecting the final suppliers. A genetic algorithm has been applied to solve the problem and a numeric example has been provided, along with sensitivity analysis, in order to validate the performance of the model. The following mathematical method provides a quantitative tool for biomass feedstock supplier selection.

2.4.1. HYPOTHESES

- The amount of demand of each strategic item is definite.
- The supply base for each commodity is fixed and is pre-determined.
- The failure rate (defect rate) of one random variable is specified with a standard normal distribution and the maximum acceptable defect rate of commodity.
- The tardiness rate (delay rate) of one random variable is specified with a standard normal distribution and the maximum acceptable delay rate.

2.4.2. DEFINITION OF PARAMETERS

D_i: Demand of i^{th} biomass feedstock.
Y_{ij}: The amount of i^{th} biomass feedstock purchased from j^{th} supplier.
X_{ij}: Binary variable (0 or 1) indicating selection or non-selection of j^{th} supplier for i^{th} biomass feedstock.
C_{ij}: The capacity of j^{th} supplier for supplying i^{th} biomass feedstock.
q_{ij}: Failure rate of j^{th} supplier for supplying i^{th} biomass feedstock.
q_{ia}: Maximum acceptable failure rate of i^{th} biomass feedstock.
L_{ij}: Tardiness rate of j^{th} supplier for supplying i^{th} biomass feedstock.
L_{ia}: Maximum acceptable tardiness rate of i^{th} biomass feedstock.
T: Supply base.
P_{ij}: The purchase price of i^{th} biomass feedstock from j supplier.
F_{ij}: Fixed cost (constant cost) of j^{th} supplier for supplying i^{th} biomass feedstock.
TBP: The total budget for purchasing biomass feedstock.
1-A: The probability of evaluating the considered quality, which is specified in advance by the decision maker.
1-B: The probability of evaluating the time between ordering and receiving the considered commodity.

2.4.3. THE FINAL MATHEMATICAL MODEL

The objective function is obtained by the sum of fixed and variable costs of the commodities from the selected suppliers (Eq. 1). The model considers several constraints: capacity, quality, supplies base, lead-time, demand, total amount of budget, and non-negative limitation, respectively (Eqs. 2-9).

$$Min \sum_{i=1}^{n}\sum_{j=1}^{m_i}\left(P_{ij}Y_{ij} + F_{ij}X_{ij}\right) \quad (1)$$

ST:

$$Y_{ij} \le C_{ij}X_{ij} \quad i = 1 \dots n, j = 1 \dots m_i \quad (2)$$

$$\sum_{j=1}^{m_i} X_{ij}\mu_{ij} + M\emptyset^{-1}(1 - A) \le q_{ia} \quad (3)$$

$$\sum_{j=1}^{m_i} X_{ij} \le T \quad i = 1 \dots n \quad (4)$$

$$\sum_{j=1}^{m_i} X_{ij}\mu_{ij} + N\emptyset^{-1}(1 - B) \le L_{ia} \quad (5)$$

$$\sum_{j=1}^{m_i} Y_{ij} \ge D_i \quad (6)$$

$$\sum_{i=1}^{n}\sum_{j=1}^{m_i} P_{ij}Y_{ij} \le TBP \quad (7)$$

$$X_{ij} = 0 \text{ or } 1 \quad for\ all\ i\ and\ j \quad (8)$$

$$Y_{ij} \ge 0 \quad i = 1 \dots n, j = 1 \dots m_i \quad (9)$$

2.4.4. NUMERICAL EXAMPLE

In this section, the model is investigated through a numerical example using two methods: exhaustive search and a Genetic Algorithm. In the example, the hypothesis is that the management of a company tends to minimize the cost for suppliers in preparing a biomass feedstock. As Table 4 shows, the goal is to select the best supplier when the demand for the commodity is 90 units. Meanwhile, the supply base (number of suppliers) for the first commodity is considered to be three (T=3). The total allocated budget for preparing this biomass feedstock is $150,000.

Table 4. Supplier information for biomass feedstock supply chain.

Items	Price ($)	Constant cost ($)	Capacity (Ton)	Failure rate	Tardiness rate
Supplier No. 1	800	1000	80	N (0.0040,0.050)	N (0.0024,0.065)
Supplier No. 2	900	750	70	N (0.0034,0.055)	N (0.0049,0.055)
Supplier No. 3	880	950	75	N (0.0044,0.065)	N (0.0040,0.050)
Supplier No. 4	900	800	65	N (0.0040,0.055)	N (0.0040,0.050)
The demand for this commodity is 90 units				q_{1a} =0.15	L_{1a} =0.2
The maximum number of suppliers is 3 (T=3)				1-A=0.85	1-B=0.8

2.4.5. *SOLVING THE MATHEMATICAL MODEL*

For the given commodity with four suppliers, there are 16 cases for selecting suppliers; and, as indicated in Table 5, feasibility or infeasibility is determined based on the demand and the amount of the commodity supplied.

Table 5. Example of solutions satisfying demand and amount supplied (Constraints 2, 6).

Case	Supplier No. 1	Supplier No. 2	Supplier No. 3	Supplier No. 4	Amount (Y_{ij})	Feasibility
1	1	1	1	1	290	Feasible
2	1	1	1	0	225	Feasible
:	:	:	:	:	:	:
15	0	0	0	1	65	Infeasible
16	0	0	0	0	0	Infeasible

Among the feasible cases explored using the exhaustive search technique (evaluating and comparing all possible scenarios), the best case is shown in Table 6. It is seen that the first and third suppliers are selected. The lowest cost for two suppliers is equal to $74,750. It is possible to realize the feasibility of the solution based on the limitations of supply capacity and demand of this commodity due to the low number of suppliers. In larger problems, however, this decision will be very difficult because, in addition to the two selection limitations (quality and lead-time), there are stochastic constraints. Therefore, this model is constituted as NP-hard. The Genetic Algorithm (GA) is applied to solve this model, which is a common approach to solving NP-hard models [24]. Table 6 also indicates the GA solution from MATLAB, and shows that the first and the fourth suppliers have been selected with this approach. The best and the least cost for supplying this strategic commodity is $74,900, which is less than the initial solution.

Table 6. Comparision of solutions (units purchased and overall cost) using two methods.

Methods	Supplier No. 1	Supplier No. 2	Supplier No. 3	Supplier No. 4	Overall Cost
Exhaustive Search	80	0	10	0	$74,750
Genetic Algorithm	79	0	0	11	$74,900

One reason for the difference between these two solutions is due to the stochastic constraints. The exhaustive search satisfies the stochastic constraints to find a feasible solution GA satisfies not only the stochastic constraints, but also selects the supplier (# 4) exhibiting lower variance. To clarify, variance is a measure of uncertainty or, as in this problem, quality.

The overall cost of the numerical example obtained by the exhaustive search method and the GA method are very close (within $150, or a 0.1% difference). Figure 4 indicates the evaluation of objective function (cost) for the GA iterations. The top graph shows the cost for each consecutive generation. It shows that the algorithm quickly reaches the optimum value (after 20 generations). The bottom graph is related to the objective function, where the solid line indicates the optimum cost and the dashed line indicates the mean cost in each generation.

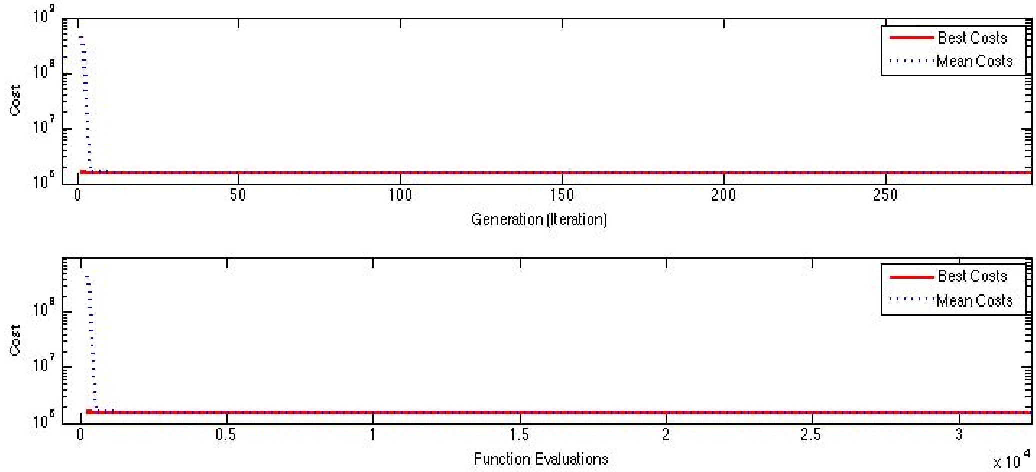

Figure 4. Genetic Algorithm cost results, Top: For each generation and Bottom: For function evaluations (MATLAB result).

2.4.6. Sensitivity Analysis

There are many methods for confirming mathematical optimization models. Thus, the supplier selection model can be evaluated using sensitivity analysis for three cases in future work:

- *Coefficients of basic variables in objective function:* Changes in coefficients of basic variables can influence the optimization results.
- *Coefficients of non-basic variables in objective function:* Changes in coefficients of non-basic variables should not influence the optimization results. Thus, if there is an effect methodological errors can be revealed.
- *Right hand numbers:* In the provided model, the maximum acceptable failure rate of the i^{th} biomass feedstock (q_{ia}) and the maximum acceptable tardiness rate of the i^{th} biomass feedstock (L_{ia}) are constituted as right hand numbers. The changes of this parameter can make the optimum solution of the problem feasible or infeasible.

3. Conclusions

From the above method and application, the evaluation and selection of the best supplier is obtained for a hypothetical biomass feedstock supply chain. Due to numerous biomass supply uncertainties, research to support biomass supply chain (BSC) network design requires the development of advanced methods. Biomass feedstocks greatly affect the BSC due to the impact on cost and life cycle environmental impacts. One of the most applicable approaches to select suppliers is introduced applied in this research. The first step is Problem Formulation, which defines what buyers need to achieve from suppliers. The Kraljic Portfolio Purchasing Model determines the items in four clusters simultaneously to define which kind of supplier can provide these items. The decision tree method is applied to solve this classification model. The second step is criteria definition. While more than 200 factors are introduced in the literature, four of them (price, quality, capacity, delivery time) have been primarily used in prior work. In this effort, each of these four factors was considered due to their importance in selecting a proper supplier. The third step is pre-selection of potential suppliers, which evaluates and selects the qualified supplier from all suppliers. The SVM method is provided to find potential suppliers. In the final step that is significance phase, a mathematical model is proposed with the purpose of selecting the supplier which minimizes the cost of purchasing feedstock. Since the final model has two stochastic constraints, the genetic algorithm is demonstrated to solve this model for the hypothetical example.

It is shown that this integrated machine learning and mathematical programming method offers a promising approach to supplementing existing supplier selection methods for biomass-to-biofuel supply chains. Future research must evaluate the robustness of the method, however, based on actual supply chain data. This future work will reveal the potential for agricultural development, technological advancements, and methodological approaches for ensuring viable and sustainable alternatives for conventional liquid fuels and other energy sources.

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