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RESEARCH ARTICLE

Mathematical Modeling and Optimization of Supply Chain for Bioethanol

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ABSTRACT

Biofuels today are a good solution in the tendentiously declining stocks of raw materials for conventional fuels. They are used by adding in a certain percentage to usable fuels for transport combustion systems. Their environmental performance is also a good feature in environmental protection. European and global scale, there is an increased use in the coming years, adopted in prescriptions and directives. One of these biofuels is bioethanol, which also finds other applications in the industry and bits. For this purpose, optimal supply chains (SC) are developed, including suitable raw materials, technologies and equipment. This can be done by developing a mathematical model describing the extremely large number of parameters and factors, as well as their limits for real application. Then it is necessary to conduct numerical experiments through multifactorial and multi-critical optimization. The development presents the mathematical model and its software implementation on the GAMS platform. Modeling and optimization has been carried out according to economic and environmental criteria, and the results obtained can be used to build optimal SC for a particular territory – region, state or country.

Keywords: Modeling, Optimization, Bioethanol, Supply Chain

1. INTRODUCTION

In recent years, the global population has markedly increased, resulting in a greater demand for energy and a higher consumption of petroleum fuels, which has led to the gradual depletion of reserves. Rising population also puts greater demands on the transport sector, which accounts for about 30% of total energy consumption in Europe. In turn, all of this leads to an increase in greenhouse gases released into the atmosphere. These facts motivate scientists to look for alternative energy sources, especially those derived from renewable raw materials, such as biomass. It is the only suitable and renewable primary energy resource from which alternative transport fuels such as bioethanol, biodiesel and biogas can be obtained in the short and long term (Sun et al., 2002; Hamelinck et al., 2005).

The expert group set up by the European Commission has estimated that there is great potential for biofuel production (out of the actual 2% of total fuels used, with a target of 25% in 2030) (ftp://ftp.cordis.europa.eu). In order to replace the share of fossil fuels required by Directive 2003/30 / CE (European Parliament Directive), it is permissible for the land used for biomass production to be between 4-18% of the total EU agricultural land. Sustainability assessment requires sustainable technologies for the production of biofuels from different types of raw materials. In addition, technical and economic analyses (Sassner et al., 2008) are also important to assess long-term sustainability in terms of resource consumption.

To achieve this goal, as well as to deliver a competitive product to the market, it is necessary to establish a stable, reliable, sustainable, environmentally friendly and optimal resource-supply chain (SC). The construction of such a SC can be a difficult task due to the scale and complexity of the system. SCs have great economic and environmental potential, which makes them a promising source for the production of environmentally friendly biofuels (Bowling et al., 2011). For this purpose, sustainable resource-supply chains must be established, which consider all stages of the production of the respective biofuel. Biofuel supply chains provide opportunities to improve the economic, environmental, and social performance of production systems (Harahap et al., 2020). However, careful planning of plant configuration, harvesting, production and field, and plant locations have a significant value in obtaining the maximum benefits from these systems. Likewise, feedstock availability and spatial distribution, product demand, and biofuel supply chain costs affect the overall economics of the plants, requiring proper strategy preparation to direct and promote investments over time (Gupta et al., 2020).

A bi-objective mixed-integer linear programming (MILP) model was proposed to formulate the optimal design and planning of a bioethanol supply chain network considering competition of food and biomass feedstock over the available croplands. The performance of the proposed model was demonstrated through a multi-feedstock bioethanol supply chain. From this study we can conclude that the proposed integrated land planning-network design framework outperforms hierarchical approaches in which network design and land planning problems are solved separately in a sequential manner (Rahemi et al., 2020).

Biofuels have a number of advantages over conventional fuels: They are high in calories, they are cheap and affordable, they burn less harmful oxides and they have little residual ash. Bioethanol can be produced from different types of raw materials. They are classified into three categories of agricultural biomass containing starchy materials (wheat, potatoes, cassava, corn, rice, barley and sweet potatoes), sucrose (sugar beet, sugar cane, sweet sorghum and fruit) and lignocellulosic materials (for example of straw, wood and grass). The environmental impacts caused by large-scale lignocellulosic biomass production and the economic impacts of inefficient bioenergy production from low-energy biomass feedstocks are two factors which limit the successful development of the bioenergy sector (De Meyer et al., 2014; Ko et al., 2020). Therefore, efficient management of the lignocellulosic biomass supply chain (BBSC) is essential for second-generation biofuel development projects (Sharma et al., 2013).

In recent years, bioethanol has become one of the most important biofuels, which is renewable and environmentally friendly. (Balat et al., 2008; Balat et al., 2009). Bioethanol can be used in its pure form in special hybrid engines or mixed with gasoline in various proportions. Another advantage should be noted, namely the higher octane number and higher heat of vaporization (Kim et al., 2005). It is an enriched fuel with 35% oxygen, which reduces particulate matter and nitric oxide (NOx) emissions during combustion. It is biodegradable and contributes to sustainability (Balat et al., 2009). In addition, bioethanol is also an excellent fuel for future modern hybrid vehicles.

Bioethanol-gasoline blends in the range of 5-20% can be used without any engine improvement. This mixing contributes to the increase of fuel in the combustion process (Hsieh et al., 2002). The profile of greenhouse gas emissions (CO, HC and NOx) emitted during the combustion of such mixtures is also improved by reducing CO and hydrocarbon (HC) emissions, which are the results of increased flammability of the overall combination (Hsieh et al., 2002; Najafi et al., 2009). However, CO2 emissions are increased by mixing gasoline and bioethanol, precisely because of the improved combustion (Hsieh et al., 2002). At the same time, NOx emissions vary significantly compared to clean petrol engines, but the results are usually less predictable than HC and CO measurements, with NOx generation directly dependent on the engine type (Hsieh et al., 2002).

2. AIM

The main purpose of this study is to conduct modeling and optimization of the bioethanol supply chains needed for a particular territory, region, state or country.

The optimization problem is solved using an economic criterion, as the environmental one is defined as a constraint or vice versa. The article includes a mathematical model and software implementation for multifactorial and multi-criteria optimization. The approach should be used to meet the bioethanol needs of a particular region, state or country.

3. MATHEMATICAL MODEL DESCRIPTION

We need to create mathematical models so that the created Supply Chain can work at an optimal level.

Mathematical modeling goes through the following main stages: Problem statement; Creating a mathematical model; Selection or development of a numerical method; Compiling an algorithm; Programming; Obtaining results from the model; Modeling a cycle until satisfactory results are achieved in comparison with the real modeled process or object, experiment; Implementing the results of the model in practice.

A super-structured SC for biofuels includes a set of biomass sites, a set of search areas, as well as potential locations for a number of collection facilities and biorefineries. The mathematical model is coded using GAMS software and is a decision tool.

Basic dependencies

As noted above, the assessment of the production and distribution of bioethanol (E100) has to be made on the basis of three criteria: economic, environmental and social.

- *Model of total environmental impact of Bioethanol Supply Chain (BSC)*

The environmental impact of the SC is measured in terms of total greenhouse gas emissions ($kg\,CO_2-eq$) resulting from the life-cycle activity. They are converted into carbon credits multiplied by the market price of carbon emissions ($kg\,CO_2-eq$).

The environmental objective is to minimize the total amount of equivalent greenhouse gas emissions resulting from the operation of SC. The wording of this objective is based on a “life cycle” analysis, which takes into account the stages from the biomass production to its use as liquid fuel in the transport sector and includes:

► *cultivation and harvesting of biomass,*

► *transport of biomass to processing facilities,*

► *transport of bioethanol (E100) to mixing areas and customer centers,*

► *liquid transport fuels distribution in the search areas,*

► *emissions from the use of bioethanol (E100) and petrol in internal combustion engines.*

The ecological criteria will represent the total impact on the environment during the operation of SC, through the obtained greenhouse gas emissions at each time interval. $t \in T$. These emissions are equal to the sum of the environmental impacts of each stage of the life cycle. Greenhouse gas emissions are usually determined as follows for each time interval $t \in T$:

$$TEI_t = ELS_t + ELB_t + ELD_t + ETT_t + ESW_t + ESTRAW_t + ECAR_t, \forall t \qquad (1)$$

where,

TEI_t Total GHG impact at work on BSC for each $t \in T$. [$kg\, CO_2 - eq\, d^{-1}$];

$\left\{\begin{matrix} ELS_t \\ ELB_t \\ ELD_t \\ ETT_t \end{matrix}\right\}$ Environmental impact of the life cycle stages;

ESW_t GHG impact from solid waste recovery for all time intervals $t \in T$;

$ESTRAW_t$ GHG impact generated by the utilization of residual straw in the areas for each time interval $t \in T$;

$ECAR_t$ GHG impact of Usage bioethanol and gasoline, [$kg\, CO_2 - eq\, d^{-1}$].

The environmental impact assessment at each stage of the life cycle includes:

- ELS_t *Cultivation of biomass;*
- ELB_t *Production of bioethanol (E100);*
- ELD_t *Preparation of petroleum gasoline;*
- ESW_t *Recovery of solid waste;*
- ETA_t *Transport of biomass;*
- ETE_t *Bioethanol transportation (E100);*
- ETD_t *Gasoline transportation;*
- ETW_t *Solid waste transportation;*
- ETU_t *Straw transportation;*
- ETV_t *Transportation of wheat/corn for food security;*
- $ECAR_t$ *Bioethanol (E100)and gasoline uses in vehicles* .

- *Model of total cost BSC* TDC_t, *[\$ $year^{-1}$]*

Annual operating costs include biomass cultivation costs, local fuel distribution costs, costs for production of final products, costs for transport of raw materials and final products. Production costs include fixed annual operating costs, as a percentage of total investment capital, and variable costs, which are proportional to the amount of processing. Transportation costs take into account both distance-fixed costs and distance-variable costs. The economic assessment is determined according to the total investment costs for the bioethanol production facilities (E100), the costs for the construction of the production facilities and the operation of the BSC for the period of operation. This price is expressed by the dependence (2) for each time interval $t \in T$:

$$TDC_t = TIC_t + TIW_t + TPC_t + TPW_t + TTC_t + TTAXB_t - TL_t - TS_t, \quad \forall t \qquad (2)$$

where,

TDC_t Common cost of an BSC for year [$\$ \, year^{-1}$];

TIC_t Common investment costs of production capacity of BSC per year [$\$ \, year^{-1}$];

TIW_t General investment costs of solid waste plants per year [$\$ \, year^{-1}$];

TPC_t Costs for production of biorefineries [$\$ \, year^{-1}$];

TPW_t Production cost for solid waste plants [$\$ \, year^{-1}$];

TTC_t Total costs for transportation of a BSC [$\$ \, year^{-1}$];

$TTAXB_t$ A carbon tax levied according to the total amount of CO_2 generated in the work of BSC [$\$ \, year^{-1}$];

TL_t Government incentives for bioethanol production and use [$\$ \, year^{-1}$].

TS_t Total costs of selling straw for other purposes, [$\$ \, year^{-1}$].

- *Model of social assessment of a BSC* Job_t, *[Number of Jobs]*

The IBSC Social Assessment Model is to determine the expected total number of jobs created (Job_t) as a result of the operation of all elements of the system during its operation.

$$Job_t = NJ1_t + LT_t NJ2_t + LT_t NJ3_t, \quad \forall t \tag{3}$$

The components of Eq (3) are defined according to the relations for each time interval,

$NJ1_t$ number of jobs created during the installation of bioethanol refineries and solid waste plants,

$NJ2_t$ number of jobs created during the operation of bioethanol refineries and solid waste plants,

$NJ3_t$ number of jobs created by cultivation of bioresources for bioethanol production,

LT_t Duration of time intervals [*year*]

$$\left.\begin{aligned} NJ1_t &= \sum_{p\in P}\sum_{f\in F}\left(M_{ft}^{JobP} JobB_p Z_{pft}\right) + \sum_{s\in S}\sum_{w\in W}\left(M_{wt}^{JobW} JobW_s ZW_{swt}\right) \\ NJ2_t &= \sum_{p\in P}\sum_{f\in F}\left(M_{ft}^{JobP} JobO_p ZF_{pft}\right) + \sum_{s\in S}\sum_{w\in W}\left(M_{wt}^{JobW} JobOW_s ZWF_{swt}\right) \\ NJ3_t &= \sum_{i\in I}\sum_{g\in G}\left(JobG_{ig} PBB_{igt}\right) \end{aligned}\right\}, \quad \forall t \tag{4}$$

Equations (3 and 4) represent a simplified model of the social evaluation criterion, which was first discussed in detail in **(Osmani et al., 2017).**

4. FORMULATION OF THE OPTIMIZATION PROBLEM USING THE MATHEMATICAL MODEL

The optimization procedure uses a set of decision variables, both binary and continuous, that minimize the selected objective function. The independent variables of the solution are:

- *SC structure, which includes: size, location of biorefineries and number,*
- *rate of biomass cultivation of each type and technology for bioethanol production,*
- *location of bioethanol production facilities and biomass sites,*
- *location of the facilities for utilization of the generated solid waste in the production of bioethanol,*

• *flows of each type of biomass and bioethanol between cells,*

• *modes of transport for delivery of biomass and bioethanol,*

• *greenhouse gas emissions for each stage of the life cycle,*

• *transport costs for each transport connection and transport regime,*

• *biofuel distribution processes to be sent to blending and search areas.*

4.1. The Following Model Considers Two Objective Functions that Determine:

4.1.1. Economic sustainability ($COST$ or $COST_{TBG}$): Minimization of the total logistics costs of the supply system, taking into account fixed, variable and emission costs [$]:

$$COST = \sum_{t \in T} \left(LT_t TDC_t \right) \tag{5}$$

$$COST_{TBG} = \sum_{t \in T} \left(LT_t TBG_t \right) \tag{6}$$

4.1.2. Environmental resilience (*ENV* or $Cost_{ENV}$): Minimize the total amount of greenhouse gas emissions, calculated in units of [*kg* or *$*] carbon dioxide equivalent [$kg\, CO_2 - eq$]:

$$ENV = \sum_{t \in T} \left(LT_t \; TEI_t \right) \tag{7}$$

$$Cost_{ENV} = C_{CO_2} ENV \tag{8}$$

Which *CostENV [$year*$^{-1}$*]* is the price to be paid to prevent the environmental impact of the amount of carbon dioxide equivalent, while the Global Warming Ratio [$\$ / kg\, CO_2 - eq$] (the most commonly used values are $0.135 \$ / kg\, CO_2 - eq$) is according to (Miret et al., 2016).

4.1.3. Social sustainability (*JOB*): Increasing the social impact of the systematic operation of the supply chain [*Number of Jobs*]:

$$JOB = \sum_{t \in T} \left(LT_t \; Job_t \right) \tag{9}$$

The problem for the optimal design of BSC is formulated as MILP for different target functions, as follows:

4.2. Models of Objects with One Criterion

The first approach considers that the SCM problem has only one target optimization function, which is usually an economic or environmental variable.

The strategic design of the SC integrates two levels of planning: solutions for the configuration of the SC and the task of each refinery, solutions for planning the flows of biomass and fuels in the network.

4.2.1. Minimizing greenhouse gas emissions, [*kgCO*$_2$*-eq.]*

The environmental objective is to minimize the total annual CO_2- equivalent greenhouse gas emissions resulting from the operation of the bioethanol and gasoline SC's used to ensure the energy balance of the regions. The formulation of this task is based on the total greenhouse gas emissions in the SC and other fuels are calculated based on the LCA approach, in which emissions are added throughout the life cycle.

The task for determining the optimal location of the facilities in the regions and their parameters is formulated as follows:

$$\begin{Bmatrix} Find: X_t[\text{Decision variables}]^T \\ MINIMIZE\{ENV(X_t)\} \rightarrow (Eq.7) \\ s.t.:\{subjecttopre-imposedrestrictions\} \end{Bmatrix} \tag{10}$$

The objective function (7) and the constraints (subject to pre-imposed restrictions) are linear functions with respect to all independent variables.

4.2.2. Minimize annual costs [\$]

Economic value is of the utmost importance and it is not necessary to integrate other objectives, such as environmental greenhouse gas emissions, in models based on the same objective.

The economic objective is to minimize total annual costs, including total annual capital costs, annual operating costs, annual government incentives and CO_2-issuance costs. The task for determining the optimal location of the facilities in the regions and their parameters is formulated as follows:

$$\begin{Bmatrix} Find: X_t[\text{Decision variables}]^T \\ MINIMIZE\{COST(X_t)\} \rightarrow (Eq.5) \\ s.t.:\{subjecttopre-imposedrestriction\} \end{Bmatrix} \tag{11}$$

The objective function (5) and the constraints (subject to pre-imposed restrictions) are linear functions with respect to all independent variables.

4.3. Multicriteria models

The second class formulates the strategic decisions of SC as multi-criteria (multi-purpose) models. The planning decisions are almost the same. However, additional goals are added in the optimization process.

The reference point approach uses the target values F_{ti}^{ref} found by separately solving the optimization problem for a given set of targets (5) - (9) and finding an optimal Pareto solution that minimizes the overall loss function of the reference values F_{ti}^{ref}. For example, for two purposes - total costs *MINIMIZE{COST(X_t)}* and *MINIMIZE{ENV(X_t)}* greenhouse gas emissions - the decision problem is solved as follows:

$$\begin{pmatrix} Find: X_t[\text{Decision variables}]^T \\ To\ \ MIN.: F_t(X_t) = \begin{pmatrix} COST(X_t) = Total\,\text{cost} \\ ENV(X_t) = \text{GHG Emissions} \end{pmatrix} \\ s.t.:\{subjecttopre-imposedrestrictions\} \end{pmatrix} \Rightarrow \begin{pmatrix} Find: X_t[\text{Decision variables}]^T \\ To\ \ MIN.: Z_t(X_t) = \sum_{i=1}^{2}\left(\delta_{ti}^2(X_t) w_{ti}\right) \\ s.t.:\{subjecttopre-imposedrestrictions\} \end{pmatrix} \tag{12}$$

Where $\delta_{ti}(X_t)$ are the normalized losses for each objective of the reference value F_{ti}^{ref} and w_{ti} are the weighting factors representing the priorities given for each objective.

The "ε-limitation" method is used to minimize costs while ensuring that life-cycle greenhouse gas emissions are acceptable. In this method (with inverse articulation of preferences), one goal is chosen for optimization, and the rest are reformulated as constraints:

$$\begin{pmatrix} Find: X_t[\text{Decision variables}]^T \\ To\ \ MIN.: F_t(X) = \begin{pmatrix} COST(X_t) = Total\,\text{cost}\ IBSC \\ ENV(X_t) = \text{GHG Emissions} \end{pmatrix} \\ s.t.:\{subjecttopre-imposedrestrictions\} \end{pmatrix} \Rightarrow \begin{pmatrix} Find: X_t[\text{Decision variables}]^T \\ To\ \ MIN.: F_t(X_t) = COST(X_t) \\ s.t.: \begin{Bmatrix} ENV(X_t) \le \varepsilon \\ \{subjecttopre-imposedrestriction\} \end{Bmatrix} \end{pmatrix} \tag{13}$$

By progressively changing the limits ε, which represent the greenhouse gas emission limit in this case, samples can be taken from different points on the front of the Pareto. By calculating the extremes of the Pareto front, the range of different objective functions can be calculated and the constraints can be selected accordingly.

Problems 4.1.1. and 4.1.2. are standard MILPs and can be solved using standard MILP techniques. The model was developed by the commercial software General Algebraic Modeling System (GAMS) (McCarl et al., 2008) and chooses the cheaper routes from a set of biomass supply points to a specific plant and in addition to a set of points to achieve bioethanol. The end result of the optimization problem will be a set of installations together with their respective points of biomass, bioethanol and gasoline.

5. RESULTS

The approach described above is applied for numerical modeling of Supply Chains for bioethanol for the territory of the Republic of Bulgaria. It occupies an area of 110,000 square kilometers on the Balkan Peninsula in Europe. The country is divided into 27 administrative regions (Ivanov et al., 2014), each of which has specific geographical and climatic features.

For the practical application of the approach it is necessary:

- to introduce the constant and known parameters, as well as the variables that are subject to optimization;
- to define the target functions and all restrictions;
- to introduce the time set of intervals on the planning horizon *t={1,2,..,T}*. The index t indicates the variable or parameter corresponding to the scheduling interval tth;
- to introduce the restrictions on:

  - o The capacity of the production facilities, which is restricted by the lower and upper limits:
  - o Current eligibility limit of SC
  - o Restriction guaranteeing the regions' needs for biomass for technical purposes
  - o Restriction guaranteeing the regions' needs for grain to meet food requirements
  - o Limitation of the capacities for utilization of the solid waste from the upper and lower limits
  - o Logical constraints
  - o Transport restrictions
  - o The total environmental impact of all neighboring regions
  - o The material balance for bioethanol and biomass in the regions
  - o The mass balance between bioethanol production facilities and customer consumption areas
  - o Crop rotation of crops in the region
  - o Guaranteeing the overall energy balance of the region
  - o Ensuring and guaranteeing the energy balance of each customer area
  - o Guarantee and delivery of the required amount of fuel for each region

For the successful application of the approach for numerical modeling and optimization of SC for bioethanol it is necessary to use information about the territorial and climatic features of the region (/; /; Kondili et al., 2007), with the possibilities for cultivation and use of potential raw materials (). In addition, selection of appropriate technology for bioethanol production (Lennartsson et al., 2014), location of biorefineries and gasoline warehouses, transport communications (Ivanov et al., 2013; ; http://www. europabio.org/) and specific climatic features are all matters to be taken into account. The main target functions are related to the total costs of SC for bioethanol (http://www.biofuels.apec.org/), its price to the end user and compliance with environmental standards for environmental pollutants.

Optimization problems can be formulated and solved at the following Optimization criterion: minimum amount of GHG emissions and minimum average annual costs.

In Fig. 1 presents the result of the modeling of SC for bioethanol in the territory of Bulgaria for the location and logistics of biorefineries, gasoline storages and utilization capacities in 2020 in case of minimum total annual costs.

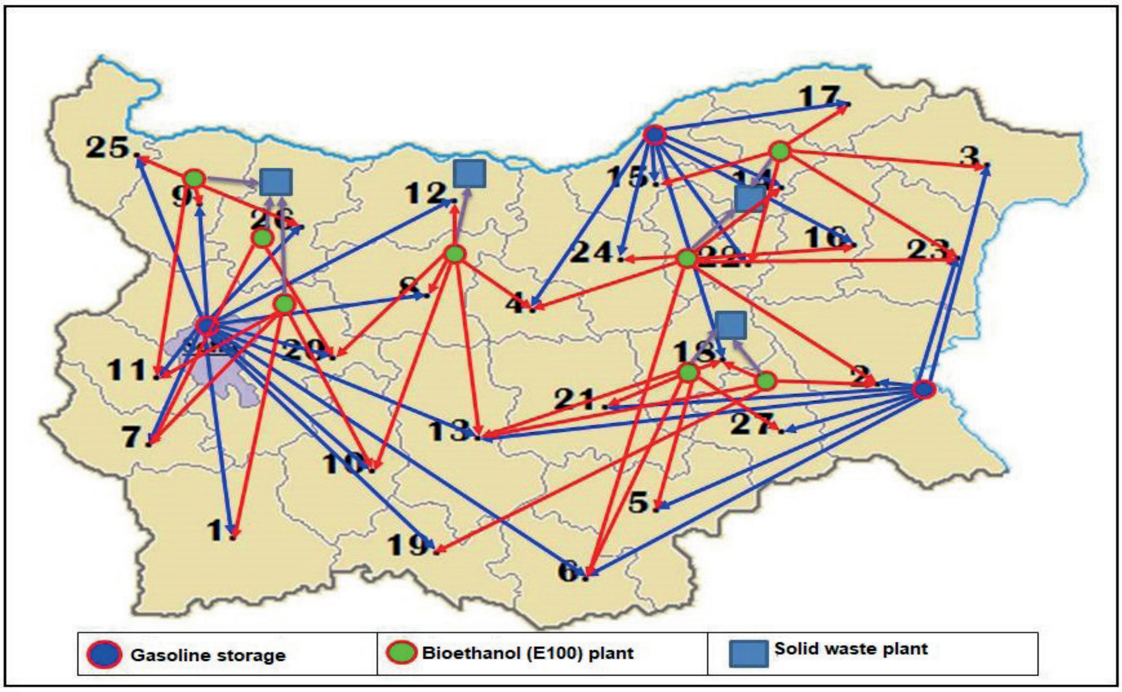

Figure 1. Optimal structure of the SC for bioethanol and logistics links in terms of the supply of bioethanol and petrol, as well as the logistics of solid waste transportation to the recycling plants for 2020.

CONCLUSION

Biofuel production is expected to develop rapidly in the coming decades because of growing environmental pollution, the inefficient use of energy and a global energy crisis. The energy future of the world is inextricably linked with the development of techniques for the controlled production of biofuels.

This paper presents an approach for a Bioethanol Supply Chain on economic and environmental criteria, taking into account the main characteristics of biofuels such as seasonality for supply of raw materials, geographic diversity and availability of biomass, other conversion technologies, recycling of by-products, distribution demand, and the regional economic situation. The presented model allows for the minimizing of economic costs and the reduction of harmful emissions released in the chain by making the necessary compromises. The design of optimal SC for biofuel can solve a wide range of issues related to biofuels because this area changes very quickly.

In this study, an approach for numerical modeling and optimization according to economic and environmental criteria of bioethanol supply chains was developed. It includes a mathematical model and its software implementation on the GAMS platform for multiparametric optimization. The approach was successfully applied to the territory of the Republic of Bulgaria and it is hoped that it can be applied to another country, state or region.

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