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# DEVELOPMENT OF A MATHEMATICAL MODEL FOR LOCATING BUTYRIC ACID-BASED BUTANOL REFINERY

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**ABSTRACT**

Deciding the location of bio refinery is an important task for management in biofuel supply and demand. This work presents a single-period deterministic model for the optimal location of butanol refinery. The developed model considers a whole system approach for butyric acid supply, butanol refinery and delivery systems. The proposed model determines where and how many refineries to be constructed and components (butyric acid and butanol) to be transported for minimizing the expected total network cost and satisfying regional demand of biofuel. The real scenario of the biofuel demand by region in South Korea is applied to validate the mathematical model. The optimization results will help to determine investment strategies for butanol production.

**Keywords:** Energy management, Renewable energy, Facility location, Butanol

## NONMENCLATURE

*Abbreviations*

| | |
|---|---|
| AD | Anaerobic digestion |
| BA | Butyric acid |
| BuOH | Butanol |
| MILP | Mixed integer linear programing |
| RFS | Renewable fuel standards |
| VFA | Volatile fatty acid |

*Symbols*

| | |
|---|---|
| R | Region |
| yr | year |

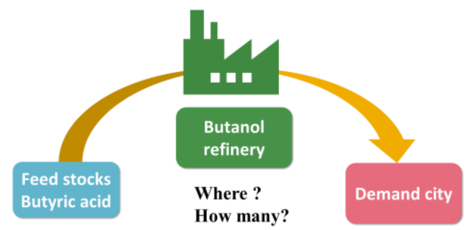



Fig 1 Overveiw of mathetical model with biorefinery location problems

## 1. INTRODUCTION

Increasing world population and industrialization have caused an explosive growth of energy demand, and also raised concerns about greenhouse gas emissions [1]. With respects to alternative fuels, renewable resources are attracting attention in an effort to supply global energy demands. The use of biofuels, such as bioethanol and biodiesel, is encouraged by political legislation like renewable fuel standards [2].

Butanol (BuOH) has considered as the alternative one of bio-fuel, and it has better properties for blending with conventional fuel including higher octane number, higher heating value, lower volatility compared to ethanol [3]. A number of researches have been conducted on butanol production from various resource [4]. BuOH can be produced from biomass by fermentation and fossil resource [5]. Recently, catalytic process for the conversion of organic waste–derived butyric acid (BA) to BuOH was reported [6]. Towards this end, the concept of BuOH refinery has been introduced to meet the increasing future energy demand.

To ensure produced BuOH satisfies energy demand, it is necessary to consider feedstock supply, effective refinery operation and biofuel distribution. Despite all the extensive research in the area of biofuel supply chain

[7], few studies have considered optimal location of bio-BuOH refinery using organic waste–derived butyric acid on large-scale.

Accordingly, we develop a mathematical model for the optimization of strategic planning of BuOH refinery. The model is formulated as a mixed integer linear programing (MILP). A real scenario based case study of production BuOH from BA in Korea is conducted. The primary goal of this work is to optimize long term, strategic decisions of BuOH refinery for the management of BA supply and BuOH demand. We aims to provide a development of a mathematical model for locating BA-derived BuOH refinery.

## 2. PROBLEM DEFINITION AND FORMULATION

### *2.1 Problem statement*

The design problem of developed model is to determine the optimal location of refineries for producing biofuel from BA and for transporting it to demand regions. The mathematical model is a MILP model. This model considers where and how many refineries to be constructed, where and how much feedstock to be transported, and BuOH to be transported to minimize the expected total network cost and satisfy regional demand under the given condition of the capacity and cost limitations of BA supply, BuOH production, BA and BuOH distribution systems (Fig 1).

### *2.2 Model formulation*

2.2.1. Objective function

The objective function aims to determine optimal location and number of BuOH refinery from sources and sinks, to minimize the expected total network cost. Total network cost is the sum of capital cost (fixed capital cost and land cost), operating cost (fixed operating cost, raw material cost and energy cost), transportation cost (pipe line transportation cost and truck distribution cost).

$$\begin{aligned} &\mathbf{min}\ f(x,y) \\ &s.t\quad h(x,y)=0 \\ &\qquad g(x,y)\le 0 \\ &\qquad x\in\mathbb{R}^n, y\in\{0,1\}^t \end{aligned}$$

*where* $f(x,y)$ is the objective function(total network cost);
$h(x,y)$ is the equality equations for system (BuOH production rate, mass and energy balances);
$g(x,y)$ is the inequality equations for system (maximum refinery capacities allowed);
$x$ represents the continuous independent variables (a number of refinery to be constructed, amounts of BA transported to refinery, amounts of BuOH transported to city);
$y$ represents the discrete independent variables (1 if refinery is constructed, 0 if equipment is not constructed);

2.2.2 Butyric acid supply

BA can be produced from the anaerobic digestion (AD) of organic wastes, however, in case of Korea, there is no large-scale AD process to generate volatile fatty acid (VFA) including BA. In this study, it is assumed that a source of BA is sewage treatment plant in Korea that processes organic wastes. Biogas contains about 66% of methane and amounts of potential BA production [8] was calculated by the ratio of methane to BA in AD process.

Table 1 Sewage treatment's biogas and BA production potentials by region in Korea

| Region | Biogas production potential ($m^3$/day) | BA production potential (ton/day) |
|---|---|---|
| R1 | 65,613 | 8,003 |
| R2 | 23,433 | 2,858 |
| R3 | 20,755 | 2,531 |
| R4 | 10,712 | 1,307 |
| R5 | 8,034 | 980 |
| R6 | 10,043 | 1,225 |
| R7 | 66,952 | 8,166 |
| R8 | 58,918 | 7,186 |
| R9 | 6,695 | 817 |
| R10 | 6,026 | 735 |
| R11 | 6,026 | 735 |
| R12 | 10,712 | 1,307 |
| R13 | 7,365 | 898 |
| R14 | 14,729 | 1,796 |
| R15 | 16,068 | 1,960 |

2.2.3 BuOH production

In this study, we consider BuOH production which based on chemical catalytic conversion using BA. In this regard, a two-step process was applied to produce BuOH from BA that can potentially be derived from AD process (Fig 2). The two-step process consists of the (1) esterification of BA to methyl butyrate and (2) hydrogenolysis of this methyl butyrate to BuOH. The previous process simulation study conducted the techno-economic analysis [6]. Based on this result, base capital and operating cost of BuOH refinery (BuOH production capacity is one millions gallon/yr) was determined and capital cost of refinery adjusted for capacity by using six-tenths rule.

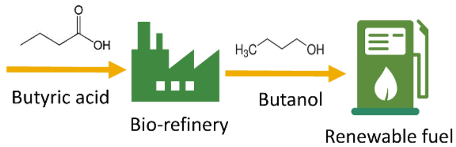



Fig2 Strategy of butanol refinery

In the butanol refinery location problem land price has a significant impact, because land costs vary widely by region [9]. The most expensive land cost of region R1 (623,303) has a price 200 times higher than the lowest cost region R9 (2,952). Land cost of refinery account for a large portion of the capital cost, so the capital cost will vary among regions.

Table2 Land price by region

| Region | Land price ($/km$^2$) | Region | Land price ($/km$^2$) |
|---|---|---|---|
| R1 | 623,303 | R9 | 2,952 |
| R2 | 84,481 | R10 | 7,160 |
| R3 | 45,949 | R11 | 6,851 |
| R4 | 59,755 | R12 | 6,800 |
| R5 | 58,724 | R13 | 4,878 |
| R6 | 48,782 | R14 | 4,276 |
| R7 | 15,917 | R15 | 8,551 |
| R8 | 33,535 | | |

2.2.4 BuOH demand

The use of biofuels is encouraged by political legislation like renewable fuel standards (RFS). According to the Korea government, transport biofuel supply expected to 0.87 million TOE by 2020 with bio-ethanol/bio-diesel ratio (33.8/66.2)[10]. In this study, we assumed the BuOH derived from BA can alternate the 3% energy demand of bio-ethanol. And biofuel demand was allocated according to the number of population by region based on real data.

2.2.5 Transportation

BA is supplied from Sewage treatment to BuOH refinery. We consider VFA as a liquid mixture which can be transported via pipeline, whose maximum length of pipe line is 250km. Delivery cost was calculated the equation including cost and energy consumption based on liquid $H_2O$ transportation [11]. And the produced BuOH was distributed by truck to demand regions. The maximum BuOH load of truck is 7800 gallon and velocity is 60 miles/hour. Transportation cost using truck includes loading and unloading cost, travel cost [9].

## 3. RESULTS AND DISCUSSIONS

### *3.1 Results and Discussion*

The case study of the Korea conducted to validate the proposed mathematical model. The model was computed using CPLEX 12.6 (GAMS) on a computer with a Intel® Core™ 3.70-GHz i7-8700K and 32 GB of RAM. Refinery location optimization results was provided in short computation time with the lowest optimal gap. For this case study, BuOH production of the model could satisfy the energy demand by region.

The optimization results for the deterministic model of BuOH refinery location was present in Table 3 and network design in Table 4. Four refineries produce bio-BuOH 3,642,011 gallons/yr, which is sufficient to replace 3% of the 2020 bio-ethanol demand. For the optimal delivery of butyric acid was influenced by delivery cost and available amount. BA produced from nine sewage treatments is supplied to 4 refineries, where BA is supplied primarily from the sewage treatment plant in the area and its insufficient amount is supplied from the adjacent sewage treatment. BuOH is distributed by demand regions with minimal transportation.

The overall network cost of BuOH is $7.312/gallon (Fig 3). The largest contributor is operating costs (52.4%) including raw material, energy cost and fixed operating cost, followed by capital cost (46.5%) including land cost. The value of total network cost increased by 13.0% compared with simulation results ($6.47/gallon) because it includes transportation and land cost. Therefore, total network cost can provide more reliable information for decision making. The developed model in this study suggests a promising strategy for biofuel production of BA-based BuOH refinery. Although it has still higher price than current market price of bio-ethanol, an optimization study of the production and separation process can improve economics of BuOH refinery. The results of this study can be applied to evaluate applicability of new biofuel production systems in real situations. And it can also be extended to a biofuel economy for a BuOH fuel station or to a future bio-BuOH supply network and energy policy.

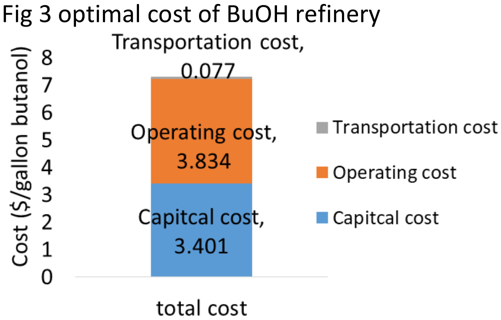
Table 3 Optimal location and production amounts of BuOH refinery by region in Korea

| Region | Number of BuOH refinery | BA production (gallon/yr) |
|---|---|---|
| R4 | 1 | 1,000,000 |
| R7 | 1 | 951,230 |
| R8 | 1 | 1,000,000 |
| R11 | 1 | 690,781 |

Table 4 Optimal BA supply network from sewage treatment and BuOH distribution network to demand region

| Region | BA supply (ton/day) | BuOH refinery | BuOH distribution (gallon/yr) | Demand region |
|---|---|---|---|---|
| R1 | 6,169 | R4 | 729,589 | R1 |
| R4 | 1,307 | | 207,942 | R4 |
| | | | 62,469 | R9 |
| R7 | 7,111 | R7 | 253,580 | R2 |
| | | | 179,918 | R3 |
| | | | 83,431 | R7 |
| | | | 194,136 | R14 |
| | | | 240,165 | R15 |
| R1 | 290 | R8 | 883,566 | R8 |
| R8 | 7,186 | | 48,478 | R9 |
| | | | 67,956 | R10 |
| R1 | 183 | R11 | 105,930 | R5 |
| R5 | 980 | | 119,728 | R6 |
| R6 | 1,225 | | 45,365 | R10 |
| R10 | 735 | | 147,816 | R11 |
| R11 | 735 | | 134,670 | R12 |
| R12 | 1,307 | | 137,273 | R13 |

Fig 3 optimal cost of BuOH refinery




## 4. CONCLUSIONS

### *4.1 Conclusions*

This study developed the deterministic model to find an optimal location for BuOH refinery. The goal of the proposed model is to minimize the total network cost of to meet the biofuel demands. The proposed model considers following approaches. 1) BA supply network via pipeline were optimized to generate enough BuOH. 2) AD process of sewage treatment were assumed that it can possible to produce BA. 3) The BuOH production process was considered to use BA via chemical catalytic conversion. 4) An optimal distribution network via truck was determined for biofuel transportation from refineries to the demand regions. A case study in the Republic of Korea evaluated the proposed model.

The results showed that locations and capacities of BuOH refineries to satisfy the biofuel demand in each regions. Also suggested optimal feedstocks delivery and bio-fuel distribution network while minimizing total network cost. As a result, we found that butanol production from butyric acid could be supplied to 3% of bio-fuel. The results suggests that it can be a promising strategy for increasing biofuel demand. New energy production and distribution can improve the future energy supply by optimizing the locations and production.

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