

# Chance Constrained Optimization of Biodiesel Supply Chain

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Biodiesel is an alternative and renewable biofuel for blending with fossil-based diesel. One of the challenges is to design the supply-chain network for biohydrodeoxygenated diesel (BHD) under uncertainty from both raw materials availability and the demand. The supply chain with four echelons; suppliers, factories, inventories and customers has been studied. The biodiesel factory has been simulated by commercial simulation program Pro/II to find the utility cost and biodiesel production capacity. In this study, the stochastic optimization is used to solve mathematical model of the BHD supply chain network. The proposed model is based on stochastic mixed-integer programming with chance constraints. The chance constrained optimization has been applied to design supply chain network under the uncertainty at different levels of confidence. Then optimized supply chain network has been investigated on stability of the supply chain network under the uncertainties, accuracy of the profit and the effect of penalty. This study shows profit and trade-off between profit and penalty cost with different levels of confidence of BHD supply chain under uncertainties in raw-material supply and biodiesel demand. The results show that the chance constrained optimization can be used to design optimum supply chain network under uncertainties within levels of confidence.

## 1. Introduction

Energy is one of the necessities in everyday life and its demand is getting higher every year. The U.S. Energy Information Administration (2019) reported that the total energy usage in 2018 was  $105.72 \times 10^9$  GJ and they predict that it will grow to  $112.50 \times 10^9$  GJ in 2050. The transportation segment is the second largest. Therefore, the sustainable energy has been concerned. The biodiesel is one of the solutions to sustain the usage of diesel in transportation segment. The first generation of biodiesel is Fatty Acid Methyl Esters (FAME) via transesterification process. However due to high oxygenated contents in this type of biodiesel, the fuel cannot be used practically as transportation fuel. The next generation of biodiesel is Bio Hydrogenated Diesel (BHD) via dehydrogenation process. This method improves fuel properties by removing oxygenated group from product (Chen et al., 2019). When production scale of biodiesel increases, the supply chain problems of uncertainty occurs (Gao and You, 2017) especially in availability of feedstock and demand for biodiesel. For the availability of feedstock, currently the main raw material for biodiesel is edible plants (Avhad and Marchetti, 2015) that share demand with food production. For the demand, biodiesel and diesel are needed for transportation fuel leading to uncertain demand of biodiesel. Therefore, the stochastic optimization is used to handle this problem. The chance constrained optimization is one of the stochastic optimization introduced by Charnes and Cooper (1959) and Miller and Wagner (1965). This method is used to find the optimum solutions under uncertainties at certain probability, in the other hand, called level of confidence.

In this work, the supply chain of biodiesel under uncertainties has been developed. The uncertainties in this model occur in suppliers and customers. The BHD plants have been simulated by process simulation software Pro/II to find correlation between feed and operation cost. Finally, the optimized supply chain has been investigated on the stability of supply chain, validation of profit and sensitivity analysis on penalty.

## 2. Methodology

The chance constrained mixed integer nonlinear programming (MINLP) has been used to optimize the supply chain of biodiesel produced from steric acid in vegetable oil. This supply chain consists of four echelons: vegetable-oil suppliers (i), BHD plants (j), BHD inventories (k) and BHD customers (l) as shown in Figure 1(a).

The objective of optimization is maximization of profit under uncertainties (at suppliers and customers) with different levels of confidence.

## 2.1 Mathematical model

The mathematical model for this supply chain is expressed as shown below.

$$\text{maximize}(ZZ) = p_{BD} \cdot \sum_k \sum_l (x_{kl} - P_l^{po}) - [ \sum_i \sum_j c_{t,ij} \cdot x_{ij} + \sum_j \sum_k c_{t,jk} \cdot x_{jk} + \sum_k \sum_l c_{t,kl} \cdot x_{kl} ] - [ p_S \cdot \sum_j x_{ij} + p_{H_2} \cdot \sum_j x_{H_2,j} + p_{HU} \cdot \sum_j HU_j + p_{CU} \cdot \sum_j CU_j + p_{EU} \cdot \sum_j EU_j ] - c_p \cdot \sum_l P_l^{ne} \quad (1)$$

s.t.

$$\sum_n C_{n,BD} \cdot (\sum_i x_{ij})^n = \sum_k x_{jk} \quad (2) \quad \Pr(\sum_k x_{kl} \geq SP_{l,rand}) \geq \beta_l \quad (8)$$

$$\sum_j x_{jk} = \sum_l x_{kl} \quad (3) \quad x_{H_2,j} = \sum_n C_{n,H_2} \cdot (\sum_i x_{ij})^n \quad (9)$$

$$\sum_k x_{jk} \geq SP_{j,av,LB} \quad (4) \quad HU_j = \sum_n C_{n,HU} \cdot (\sum_i x_{ij})^n \quad (10)$$

$$\sum_k x_{jk} \leq SP_{j,av,UB} \quad (5) \quad CU_j = \sum_n C_{n,CU} \cdot (\sum_i x_{ij})^n \quad (11)$$

$$\sum_j x_{jk} \leq SP_{k,av} \quad (6) \quad EU_j = \sum_n C_{n,EU} \cdot (\sum_i x_{ij})^n \quad (12)$$

$$\Pr(\sum_j x_{ij} \leq SP_{i,rand}) \geq \alpha_i \quad (7)$$

The objective function is to maximize profit that consists of four parts: revenue from selling BHD, transportation cost, operation cost and penalty cost as shown in Eq(1). The penalty in this model is only under demand in selling BHD or opportunity loss. However, over-demand products are not sold to customers. Eq(2) deals with mass balance and conversion of vegetable oil to biodiesel at plants. Eq(3) deals with mass balance at inventories. Eqs(4,5) deal with the minimum and maximum capacity of plants, respectively. Eq(6) deals with the maximum capacity of inventories. Eqs(7,8) deal with suppliers and customers uncertainties in terms of chance constraints at different levels of confidence ( $\alpha_i$  and  $\beta_l$ , respectively). Eqs(9-12) deal with operating utilities of plants. The chance constraints are transformed to deterministic equivalent form (Charnes and Cooper, 1959). Eq(7,8) can be rewritten to Eq(13,14) where  $\phi^{-1}$  is quantile function.

$$\sum_j x_{ij} \leq SP_{i,av} + \phi^{-1}(1 - \alpha_i) \cdot SP_{i,sd} \quad (13) \quad \sum_k x_{kl} \geq SP_{l,av} - \phi^{-1}(1 - \beta_l) \cdot SP_{l,sd} \quad (14)$$

The Eq(14) has been modified to Eq(15-17) to calculate penalty in the model.

$$\sum_k x_{kl} + P_l^{ne} - P_l^{po} \geq SP_{l,av} - \phi^{-1}(1 - \beta_l) \cdot SP_{l,sd} \quad (15)$$

$$\sum_k x_{kl} - P_l^{po} \leq SP_{l,av} - \phi^{-1}(1 - \beta_l) \cdot SP_{l,sd} \quad (16) \quad \sum_k x_{kl} + P_l^{ne} \geq SP_{l,av} - \phi^{-1}(1 - \beta_l) \cdot SP_{l,sd} \quad (17)$$

## 2.2 Biodiesel plant simulation

The kinetic models are used to calculate biodiesel produce, hydrogen, hot utility, cold utility and electric energy usage in biodiesel plant. The kinetic models of BHD process can be expressed by Arrhenius equation with constant parameters, shown in Table 1. The biodiesel plant has been simulated using kinetic models. The product specification of biodiesel is 90 % w/w purity. The simulation data of biodiesel produce, hydrogen, hot utility, cold utility and electric energy usage has been collected at different feed flow rates of steric acid then found the correlation with steric acid feed condition as shown in Figure 1(b).

Table 1 Activation energy and pre-exponential factor for kinetic model (Kumar et al., 2014).

Reaction	Ea (kJ/mol)	A <sub>0</sub> (s <sup>-1</sup> )
$C_{17}H_{35}COOH + 2H_2 \rightarrow C_{18}H_{37}OH + H_2O$	175.4	$5.57 \times 10^{12}$
$C_{18}H_{37}OH \rightarrow C_{17}H_{36} + H_2 + CO$	250.0	$1.34 \times 10^{21}$
$C_{18}H_{37}OH + H_2 \rightarrow C_{18}H_{38} + H_2O$	190.9	$4.77 \times 10^{13}$
$C_{18}H_{37}OH + 2H_2 \rightarrow C_{15}H_{32} + C_3H_8 + H_2O$	387.7	$5.08 \times 10^{32}$
$C_{18}H_{37}OH + 2H_2 \rightarrow C_{16}H_{34} + C_2H_6 + H_2O$	377.2	$1.08 \times 10^{32}$

Steric acid is  $C_{17}H_{35}COOH$  BHD is  $C_{15}H_{32}$ ,  $C_{16}H_{34}$ ,  $C_{17}H_{36}$  and  $C_{18}H_{38}$

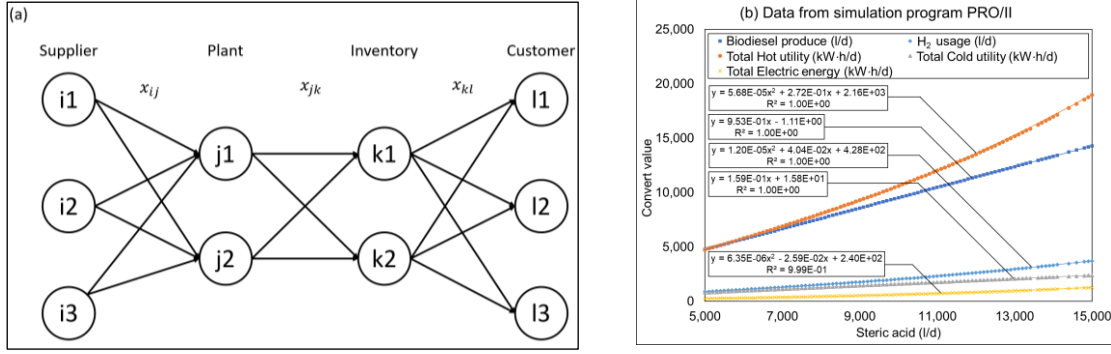


Figure 1: (a) The supply chain diagram for this work. (b) Correlation of utility data from simulation program Pro/II

### 2.3 The investigation on optimized supply chain network

The optimized supply chain network has been investigated on validation of profit, stability of supply chain and sensitivity analysis on penalty lost. The stability of network can be obtained from non-violation condition in chance constraints; Eqs(7,8) where  $SP_{l,rand}$  and  $SP_{l,rand}$  are randomly generated based on normal distribution data of steric acid availability and BHD demand, respectively. Then the levels of confidence of suppliers and customers are validated from total number of feasible data points over total number of random data points.

The validation of the optimized supply chain network can be hard to solve because the optimized supply chain network can be infeasible for example the random capacity of supplier can be less than the required value in optimized network. This leads to error in the calculation. Therefore, the network needs to recalculate from the initial state. The validation model can be expressed as shown below.

$$\max(zz) = p_{BD} \cdot \sum_k \sum_l (x_{r,kl} - P_l^{po}) - [\sum_i \sum_j c_{t,ij} \cdot x_{r,ij} + \sum_j \sum_k c_{t,jk} \cdot x_{r,jk} + \sum_k \sum_l c_{t,kl} \cdot x_{r,kl}] - [p_s \cdot \sum_j x_{r,ij} + p_{H_2} \cdot \sum_j x_{H_2,j} + p_{HU} \cdot \sum_j HU_j + p_{CU} \cdot \sum_j CU_j + p_{EU} \cdot \sum_j EU_j] - c_p \cdot \sum_l P_l^{ne} \quad (18)$$

s.t.

$$\sum_n C_{n,BD} \cdot (\sum_i x_{r,ij})^n = \sum_k x_{r,jk} \quad (19) \quad \sum_k x_{r,kl} + P_l^n \geq SP_{l,rand} \quad (27)$$

$$\sum_j x_{r,jk} = \sum_l x_{r,kl} \quad (20) \quad x_{H_2,j} = \sum_n C_{n,H_2} \cdot (\sum_i x_{r,ij})^n \quad (28)$$

$$\sum_k x_{r,jk} \geq SP_{j,av,LB} \quad (21) \quad HU_j = \sum_n C_{n,HU} \cdot (\sum_i x_{r,ij})^n \quad (29)$$

$$\sum_k x_{r,jk} \leq SP_{j,av,UB} \quad (22) \quad CU_j = \sum_n C_{n,CU} \cdot (\sum_i x_{r,ij})^n \quad (30)$$

$$\sum_j x_{r,jk} \leq SP_{k,av} \quad (23) \quad EU_j = \sum_n C_{n,EU} \cdot (\sum_i x_{r,ij})^n \quad (31)$$

$$\sum_j x_{r,ij} \leq SP_{i,rand} \quad (24) \quad x_{r,ij} + R_{ij} = x_{s,ij} \quad (32)$$

$$\sum_k x_{r,kl} + P_l^{ne} - P_l^{po} \geq SP_{l,rand} \quad (25) \quad x_{r,jk} + R_{jk} = x_{s,jk} \quad (33)$$

$$\sum_k x_{r,kl} - P_l^p \leq SP_{l,rand} \quad (26) \quad x_{r,kl} + R_{kl} = x_{s,kl} \quad (34)$$

$$M \cdot (y_i - 1) \leq SP_{i,rand} - \sum_j x_{s,ij} \leq M \cdot y_i \quad (35)$$

$$y_i (\sum_j (x_{r,ij} - x_{s,ij})) + (1 - y_i) (\sum_j (x_{r,ij} - SP_{i,rand})) = 0 \quad (36)$$

Eqs(19-31) show the modification from the chance constrained model. Eqs(32-36) deal with recalculating the initial optimized supply chain network (subscript s) to valid supply chain network (subscript r). Therefore, the valid values can be used to calculate the validated profit. Finally, the sensitivity analysis is used to see penalty cost of opportunity loss affecting on profit at different levels of confidence. This data can be obtained by varying

penalty cost of opportunity loss with the same prices and costs then compare the validate profit at different levels of confidence.

### 3. Result and discussion

#### 3.1 An illustrative example

The hypothetical case is provided to show the effectiveness of model. Table 2 shows statistical data related to capacity of suppliers, plants, inventory and demand of customers. Table 3 shows steric acid price, operation cost, penalty cost and biodiesel price. Table 4 shows transportation cost in dollar per litter.

Table 2 Data related to capacity and demand.

		Supplier			Plant		Inventory		Customer		
		i1	i2	i3	j1	j2	k1	k2	l1	l2	l3
Average Capacity or Demand (L/d)	UB:	10,000	12,500	9,500	8,000	15,000	15,000	10,000	-	-	-
	LB:	-	-	-	5,000	6,000	-	-	3,000	7,500	5,000
Standard Deviation (L/d)		1,000	1,250	950	-	-	-	-	300	750	500

Table 3 Fluid price, utility cost and penalty cost

Fluid price		Utility cost		Penalty cost		
Steric acid	20 \$/L	Hot utility		5 \$/kWh	Opportunity loss	62.375 \$/L
Hydrogen	5 \$/L	Cold utility		2.5 \$/kWh	Over-demand loss	0 \$/L
Biodiesel	49.9 \$/L	Electric energy		1.25 \$/kWh		

Table 4 Transportation cost in dollar per litter

Transportation cost from supplier to plant (\$/L)			Transportation cost from plant to inventory (\$/L)			Transportation cost from inventory to customer (\$/L)			
	j1	j2		k1	k2		l1	l2	l3
i1	2	4	j1	3	1	k1	2	3	2
i2	3	5	j2	2	4	k2	1	4	2
i3	1	3							

#### 3.2 Optimization of biodiesel supply chain network results

Figure 2(a) shows result of optimized network by chance constrained optimization at different levels of confidence. The total value of each bar represents the revenue for each case. The level of confidence of 0.50 is representative of deterministic optimization. The results show that the higher profit can be obtained at higher levels of confidence for each suppliers and customers as shown in Figure 2(a). This happen because the capacity for each supplier decreases but the BHD demand increases above the average value when using the deterministic equivalent form from Eqs(13,14). Therefore, the required quantity of biodiesel in supply chain increases, resulting in increases of BHD revenue and total cost increase.

For the validation part of optimal supply chain, the average validated profit is lower than the optimized profit as shown in Figure 2(b). This comes from the deterministic equivalent chance constrained model which does not calculate the penalty quantity (both of opportunity loss and over-demand loss) in the system. When deterministic equivalent form is used, the uncertain values are converted to certain value. Therefore, the model trends to satisfy the constraint at the new certain value and does not have penalty quantity in the network. The validation model is used to handle this problem.

Next, the trend of validated profit becomes lower at higher level of confidence. This comes from the over-demand loss is affected the revenue even though the penalty cost for over-demand loss is 0 \$/L. At higher levels of confidence for each suppliers and customers, the total quantity of biodiesel in network increases. Therefore, more biodiesel is flowing through the network but the revenue stays the same due to the over-demand products. The transportation and operation costs are higher in contrast of the penalty cost due to more biodiesel in the network. Although, the opportunity loss is lower but not trade-off with other costs. The trend of profit is going down at higher level of confidence. This case study shows that chance constrained programming only gives lower opportunity loss than deterministic programming. To improve the profit of chance constrained supply chain, the sensitivity analysis of penalty cost for opportunity loss will be done in next part.

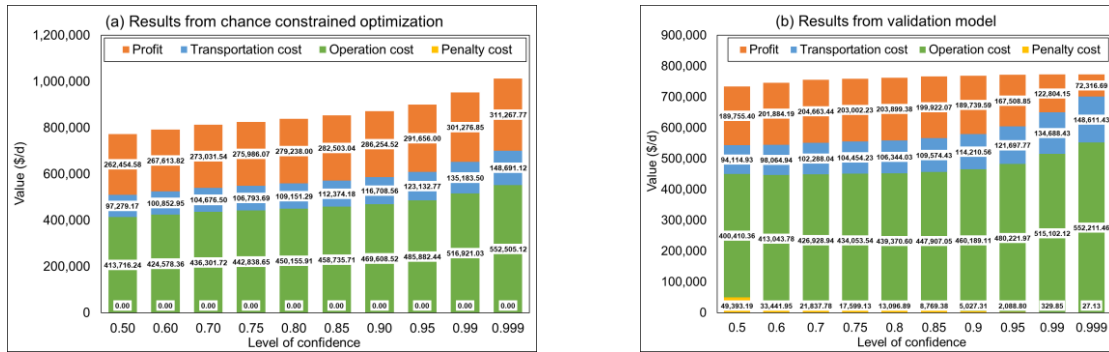


Figure 2: The results from (a) chance constrained model (b) validation model.

3.3 Feasibility of network and sensitivity analysis on penalty cost

The next investigation is to study the feasibility of constraints; Eqs(7,8) as shown in Figure 3(a). The values of levels of confidence for each supplier and customers from the stability test are away or align on the diagonal line of the graph in Figure 3(a). This means that the calculated level of confidence is greater than or equal to the level of confidence used in Eqs(7,8). This proves that the chance constrained optimization can find the optimized supply chain satisfying the condition of level of confidence.

Figure 3(b) shows the result of sensitivity analysis on penalty cost for opportunity loss. The result shows that deterministic supply chain has higher slope than chance constrained ones and their slope decreases when level of confidence increases and when the penalty cost for opportunity loss becomes larger value, the deterministic supply chain will become less profitable than chance constrained ones. For this study, at 62.375 \$/L penalty cost for opportunity loss, the penalty cost is smaller than the other costs meaning that the decrease of opportunity loss from chance constrained programming is meaningless. However, when the penalty cost for opportunity loss keeps increasing, the penalty cost and the decrease of the quantity of opportunity becomes more relevant. At 83.17 \$/L penalty cost for opportunity loss, deterministic supply chain gives profit of 196,323.27 \$/d down from 210,327.65 \$/d which is lower than chance constrained supply chain at 0.80 level of confidence which gives 210,159.77 \$/d. Furthermore, at 124.75 \$/L penalty cost for opportunity loss, deterministic supply chain gives profit of 168,314.53 \$/d which is much lower than chance constrained supply chain at 0.80 level of confidence that gives 202,311.33 \$/d.

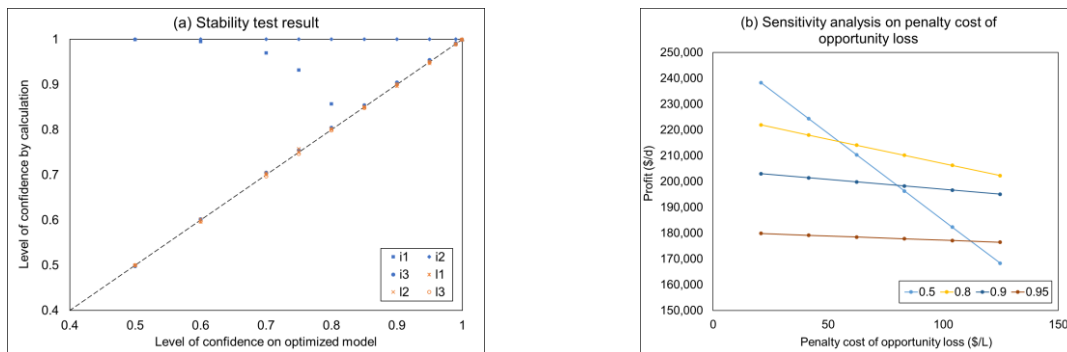


Figure 3: The result on (a) stability of supply chain (b) sensitivity analysis on penalty cost of opportunity loss.

The supply chain system designed at lower level of confidence gives more opportunity loss. Therefore, the supply chain by deterministic optimization has more opportunity loss than one by the chance constrained optimization which has higher level of confidence. The opportunity loss is the main factor that affects the sensitivity of penalty cost in this study. Therefore, higher opportunity loss in the system means that more sensitive to penalty cost. For this case study, at penalty cost for opportunity loss of 83.17 \$/L, the chance constrained optimization with level of confidence of 0.80 can improve the profit from deterministic optimization as shown in Figure 3(b).

#### 4. Conclusions

The basic concept of chance constrained programming is used to design the optimum BHD supply chain network under the uncertainties within certain levels of confidence. However, the validation step is needed to reflect the real profit value by using the result from the deterministic equivalent solving method and transform into the validated result under the uncertainties. The validated result shows that more stable network with less profit is obtained when the level of confidence increases. For this case, the deterministic optimization gives more profit than chance constrained optimization but less stability due to more opportunity loss occurring in the system. Finally, the sensitivity analysis shows that the chance constrained optimization is less sensitive to penalty cost due to the less opportunity loss occurring in the system. Therefore, the chance constrained optimization helps increase the profit of supply chain compared to one obtained from deterministic optimization when the penalty cost for opportunity loss has the significant value on the network. Further research can be conducted by improving on the accuracy on the result of the chance constrained programming when compared with validation step or using the joint probability chance constraint instead.

#### Nomenclatures

Set			
$i$	Set of suppliers	$k$	Set of inventories
$j$	Set of plants	$l$	Set of customers
Subscript			
$rand$	The random value	$H_2$	For hydrogen
$av$	The average value	$BD$	For biodiesel
$sd$	The standard deviation value	$HU$	For hot utility
$UB$	Upper bound	$CU$	For cold utility
$LB$	Lower bound	$EU$	For electric energy
$S$	For steric acid		
Parameter			
$p$	Price per litter	$C_n$	Correlation coefficient
$c_t$	Transportation cost per litter	$n$	Correlation order
$c_p$	Opportunity lost per litter	$x_s$	Optimized supply chain network
$SP$	Capacity or demand value	$M$	Large number
$\alpha/\beta$	Levels of confidence		
Variable			
$x$	Quantity in supply chain network	$x_r$	Validated supply chain network
$P_l^{po}$	Over-demand penalty quantity	$R$	Remainder in network
$P_l^{ne}$	Opportunity lost quantity	$y$	Decision variable for validation model

#### Acknowledgments

Authors would like to thank Thai Government budget fund and the Petroleum and Petrochemical College, Chulalongkorn university for financial support throughout the duration of this research.

#### References

- Avhad M. R. and Marchetti J. M., 2015, A review on recent advancement in catalytic materials for biodiesel production, *Renewable and Sustainable Energy Reviews*, 50, 696-718.
- Charnes A. and Cooper W. W., 1959, Chance-Constrained Programming, *Management Science*, 6(1), 73-79.
- Chen S., Zhou G. and Miao C., 2019, Green and renewable bio-diesel produce from oil hydrodeoxygenation: Strategies for catalyst development and mechanism, *Renewable and Sustainable Energy Reviews*, 101, 568-589.
- Gao J. and You F., 2017, Design a sustainable supply chain under uncertainty using life cycle optimisation and stochastic programming, *Chemical Engineering Transactions*, 61, 151-156.
- Kumar P., Yenumala S. R., Maity S. K. and Shee D., 2014, Kinetics of hydrodeoxygenation of stearic acid using supported nickel catalysts: Effects of supports, *Applied Catalysis A: General*, 471, 28-38.
- Miller L. B. and Wagner H., 1965, Chance-constrained programming with joint constraints, *Operations Research*, 13(6), 930-945.
- U.S. Energy Information Administration, 2019, Energy consumption by sector and source, <[www.eia.gov/outlooks/aeo/data/browser/#/?id=2-AEO2019&cases=ref2019&sourcekey=0](http://www.eia.gov/outlooks/aeo/data/browser/#/?id=2-AEO2019&cases=ref2019&sourcekey=0)> accessed 01.03.2019.