

# Bilevel Optimization for Design and Operations of Non-cooperative Biofuel Supply Chains

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We propose a bilevel mixed-integer nonlinear programming (MINLP) model for the optimal investment of biorefinery facilities considering non-cooperative farmers and biofuel consumers. Interactions among the supply chain players are captured through a single-leader-multiple-follower Stackelberg game under the generalized Nash equilibrium assumption. Given a three-echelon superstructure, the lead biofuel company in the middle echelon first optimizes its design and operational decisions, including facility location, sizing, and technology selection, material input/output and price setting. The following farmers and biofuel consumers in the upstream and downstream then optimize their transactions with the biofuel company to maximize their individual profits. Novel solution strategies are also proposed to solve the proposed bilevel MINLP efficiently. A county-level case study is presented to demonstrate the application of our model, as well as the performance of the proposed solution strategy.

## 1. Introduction

Most existing works on biofuel supply chain optimization assume that the management over the entire supply chain is centralized (Akgul et al., 2013). However, the entities in a biofuel supply chain can be in the charge of different players in practice (Yeh et al., 2014), leading to decentralized management (Bai et al., 2012). These players might not collaborate with each other and would act selfishly towards their own profit (Ryu et al., 2004). Therefore, our goal is to develop a modeling and optimization framework to assist the biofuel company's investment decision-making in such non-cooperative supply chains.

There are two major challenges towards our goal. The first challenge is how to define and model the relationships between the multiple players in the supply chain, since a monolithic model is no longer capable to capture the non-cooperative behaviors of the players. The second challenge is how to efficiently solve the resulting optimization problem, since it would involve multi-level optimization, discrete decisions, and nonlinearities in the model. To overcome these challenges, we

- propose a novel bilevel mixed-integer nonlinear programming (MINLP) model for the design and strategic planning in non-cooperative supply chains;
- extend Stackelberg game and generalized Nash equilibrium to model the relationship between the players in multi-echelon supply chains;
- develop efficient global optimization strategies for the bilevel MINLP using the KKT transformation and the successive piecewise approximation algorithm

The rest of this paper is organized as follows. We present the problem statement in Section 2. The bilevel programming model formulation is presented in Section 3, followed by the solution strategies in Section 4. A case study is given in Section 5, with results and discussions.

## 2. Problem statement

As shown by the three-echelon superstructure in Figure 1, we consider three types of players, namely a set of individual farmers, one biofuel company, and a set of individual biofuel consumers. Since the biofuel company usually has advantages in terms of resources and technologies, we assume the biofuel company to be the

leader of the supply chain, while the farmers and biofuel consumers are assumed to be followers. The biofuel company makes facility investment decisions first given the candidate sites in the middle echelon, and will be in charge of all the biorefineries to be installed. Individual farmers/consumers then respond to the biofuel company's decisions by optimizing their transactions with the installed biorefineries to maximize their own profits. This relationship between the biofuel company and the farmers/consumers can be modeled as a Stackelberg game with a single leader and multiple followers (Von Stackelberg et al., 2010). We also note that each farmer/consumer might compete their peers for certain common resources or limited quotas released by the biofuel company. We adopt the assumption of normalized Nash equilibrium to model the relationship between the followers (Facchinei and Kanzow, 2007). The optimization problems of the three types of players in the non-cooperative biofuel supply chain are formally stated as follows.

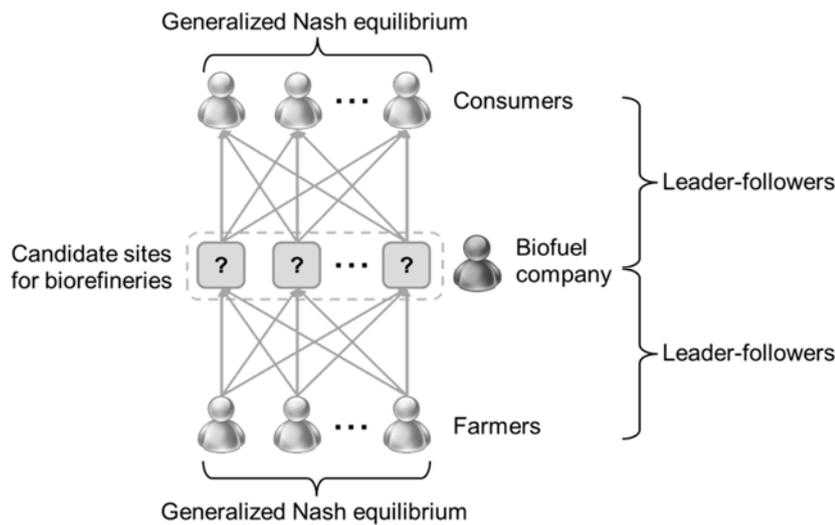


Figure 1: Superstructure of the non-cooperative biofuel supply chain.

## 2.1 Biofuel company's problem

The objective of the biofuel company is to maximize the total profit generated from all its biorefineries.

Given information to the biofuel company includes: a set of candidate locations for building biorefineries; a set of available biomass-to-biofuel technology options; restrictions on the number of biorefineries, process capacity, etc.; planning horizon and project lifetime; cost data on capital investment, operations and maintenance (O&M), etc.; restrictions on biomass/biofuel transfer prices.

Decision variables of the biofuel company include: selection of location, capacity and conversion technology for biorefineries; strategic plans on the amount of biomass to collect and the amount of biofuel to produce; setting of transfer prices for biomass acquisition and biofuel sales.

## 2.2 Individual farmer's problem

The objective of each farmer is to maximize own profit from biomass exchanges.

Given information to each farmer includes: all of the biofuel company's decisions; available amount of biomass that can be offered to the biorefineries; cost data on biomass preparation, transportation from the farmer to the biorefineries, etc.

Decision variable of each farmer is the amount of biomass sold to each installed biorefinery.

## 2.3 Individual biofuel consumer's problem

The objective of each biofuel consumer is to maximize own profit from biofuel exchanges.

Given information to each biofuel consumer includes: all of the biofuel company's decisions; local demand and market price of the biofuel product; cost data for transporting biofuel from biorefineries to the consumer.

Decision variable of the biofuel consumer is the amount of biofuel to purchase from each installed biorefineries.

A critical feature of this decentralized game-theoretic model is that the decisions of each player in the supply chain are solely driven by its own economic interest. It is worth pointing out that, from the biofuel company's

perspective, the price levels for biomass acquisition and biofuel sales must be carefully determined. If the biomass acquisition price is set too low, the farmers might refuse to sell to the biorefineries as the transaction would not be profitable. On the other hand, if the price is set too high, the biofuel company would pay unnecessary costs. The situation is similar on the biofuel consumer side. If the biofuel sales price is set too high, the biofuel consumer might be reluctant to purchase from the biorefineries due to the negative profit margin. On the other hand, if the price is set too low, the biofuel company is losing potential revenue.

### 3. Model formulation

According to the problem statement above, this is a single-leader-multiple-followers Stackelberg game with generalized Nash equilibrium assumption between the followers. We propose the following bilevel MINLP to capture the non-cooperative behaviours of the players in the supply chain.

$$\max_{x \in \mathfrak{R}^n \cup \{0,1\}} \left\{ F(x, y) \mid G(x, y) \leq 0, y^v = \arg \max_{y^v \in \mathfrak{R}^m} \left\{ f^v(x, y) \mid g^v(x, y^v, y^{-v}) \leq 0 \right\} \right\} \quad (1)$$

The lead biofuel company's decisions are denoted by vector  $x$ , which can involve both discrete variables (e.g. those for facility location and technology selection) and continuous variables (e.g., those for production planning and transfer prices). Let the followers (namely, farmers and biofuel consumers) be indexed by  $v$ . The decisions of follower  $v$  are denoted by  $y^v$ . Vector  $y^{-v}$  stands for the decisions taken by the followers other than  $v$ . Vector  $y$  is a collection of the decisions of all the followers at Nash equilibria, which involves only continuous variables (e.g., those for material exchanges). In the lower-level problems, every follower strives to maximize its own benefit function subject to its own constraints, given the leader's decisions  $x$  and other players' decisions  $y^{-v}$ . In the upper-level problem, the leader's objective function and constraints are influenced not only by its own decisions  $x$ , but also by the equilibrium decisions of all the followers  $y$ . Without loss of generality, the lower-level problems are linear programs (LPs) and the upper-level problem is a nonconvex MINLP. The nonlinearities result from the concave and bilinear terms in the biofuel company's objective function. The concave terms captures the economies of scale in the capital cost of building biorefineries. The bilinear terms are the transaction payments equal to the product of transfer prices and amount of biomass/biofuel transfer.

## 4. Solution strategies

### 4.1 KKT-condition-based reformulation

The above bilevel MINLP model cannot be directly handled by any off-the-shelf mathematical programming solvers. Therefore, we continue to reformulate the bilevel problem into a single-level MINLP. This is accomplished by replacing the lower level LP problems with their KKT conditions. Every follower  $v$ 's optimization problem is replaced by four sets of constraints, namely stationarity, primal feasibility, dual feasibility, and complementary slackness. The first three sets of constraints are linear, and the bilinear terms in the complementary slackness constraints can be linearized by introducing a set of binary variables. KKT-condition-based reformulation is a standard approach in bilevel programming and more details can be found in the book by Bard (1998). Since the lower level problems are LPs, the KKT conditions are sufficient and necessary. Therefore, the resulting single-level MINLP problem is equivalent to the original bilevel MINLP.

### 4.2 Successive piecewise approximation algorithm

Although off-the-shelf global optimizers can be used to solve the above nonconvex single-level MINLP problem, their computational performance is somewhat lacking. To further facilitate the solution of the above nonconvex MINLP problem, we introduce the successive piecewise approximation algorithm in this section. The algorithm takes advantage of the powerful MILP solvers (e.g., CPLEX) and returns the global optimal solution to the nonconvex MINLP problem by iteratively solving a sequence of MILP subproblems. Compared with its predecessor (You and Grossmann, 2011), the proposed algorithm is improved in the following two aspects. First, a new type of piecewise linear approximations based on the SOS1 variables is employed to formulate the MILP subproblems. Second, bivariate partitioning for bilinear terms is used.

An important step of the successive piecewise approximation algorithm is to iteratively construct convex relaxation problems (MILP subproblems) based on the piecewise linear approximations for the nonconvex terms, namely the concave and bilinear terms in this model. The piecewise linear approximations are derived based on the SOS1 formulation summarized in the work by Padberg (2000). By definition, at most one

variable within an SOS1 can have a non-zero value. A number of MILP solvers allow the use of SOS1 variables (e.g., CPLEX) and have certain internal routines for solving the SOS1 formulations efficiently (Hasan and Karimi, 2010). We note that grid partitioning has a great influence on approximation error (Garcia and You, 2015). Therefore, we propose a successive piecewise approximation algorithm which automatically determines the grid propagation and effectively converge within finite iterations. The procedure of the algorithm is shown in Figure 2, which is based on the work by Bergamini et al. (2008).

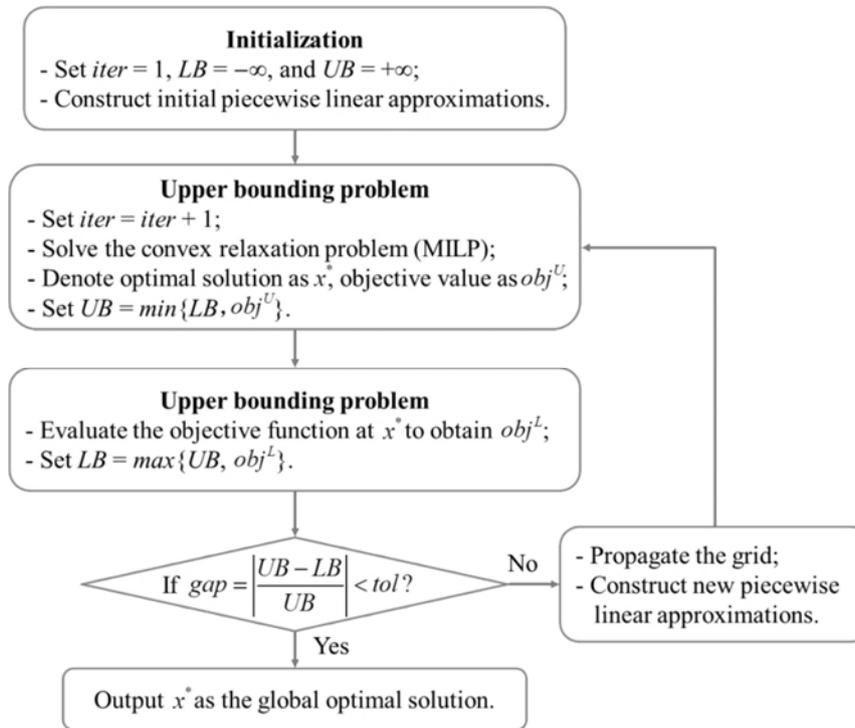


Figure 2. Flowchart of the successive piecewise approximation algorithm

## 5. Case study

Biomass-derived transportation fuels are considered a promising solution to our heavy dependence on fossil fuels and the related issues on climate change, waste pollution, energy security, and resource depletion (Yue et al., 2014). A variety of biomass can be used as feedstocks, including agricultural crops, forest residues, municipal wastes, algae biomass (Gong and You, 2014), etc. A spectrum of biofuels can be produced, including methanol, ethanol, biodiesel, drop-in hydrocarbon biofuels, etc. Besides, value-added biochemical can be co-produced to generate extra revenue (Gong and You, 2015). A number of biomass-to-biofuel conversion technologies have been developed and optimized (Gebreslassie et al, 2013), in terms of both economic and environmental performances (Wang et al., 2013). There are several contributions to the issues on sustainability (Yue et al., 2013), risk management (Tong et al., 2014), and collaboration in biofuel supply chains (Yue and You, 2014).

To illustrate the application, we present a county-level case study on the design and strategic planning of a potential cellulosic biomass-to-ethanol supply chain in the state of Illinois. The state of Illinois comprises 102 counties. We identify 10 individual farmers, 5 candidate sites for building biorefineries, and 10 individual consumers assuming that they are located at the centers of the counties (You and Wang, 2011). We consider corn stover as the biomass feedstock and ethanol as the biofuel product. The spatial distribution of corn stover availability is shown in Figure 3a. The population density is shown in Figure 3b, and we assume that the biofuel demand at each consumer is proportional to the population of that county (You et al., 2012). There are 2 biomass-to-biofuel technology options available for choice, namely the biochemical and thermochemical pathways (Sharma and Romagnoli, 2011). The biochemical conversion process is based on dilute-acid pretreatment and enzymatic hydrolysis processes, and the thermochemical conversion process involves indirect gasification and mixed alcohol synthesis. The biomass and biofuel are assumed to be shipped by truck. Considering the length of the paper, the detailed input data and mathematical model are not included but available upon request.

The optimal design that maximizes the biofuel company's profit in the non-cooperative supply chain is presented in Figure 3. The optimal design decisions made by the biofuel company are to build two biorefineries in the Champaign County and LaSalle County, respectively. The biorefinery in Champaign County has a capacity of 130 million gallons/year with the thermochemical technology. It receives corn stover from the farmers in Champaign, Iroquois, McLean, and Vermilion. The biomass acquisition cost is set at \$69.35/dry ton. It sells the produced fuel ethanol to the consumers in Champaign, Cook, Madison, St. Clair, and Will. The biofuel sales price is set at \$2.39/gallon. The biorefinery in LaSalle County has a capacity of 139 MM gallons/year with the thermochemical technology. It receives corn stover from the farmers in Bureau, LaSalle, Lee, and Livingstone. The biomass transfer price is set at \$65.14/dry ton. It sells the produced fuel ethanol to the consumers in Cook, Dupage, Kane, Lake, McHenry, and Winnebago. The biofuel transfer price is set at \$2.42/gallon. The total profit generated from the two biorefineries is \$126.68 million. The adjusted profits of the farmers range from \$0 to \$11.58 million. The adjusted profits of the consumers range from \$0 to \$2.04 million. The total profit of the entire supply chain is equal to \$158.00 million. We can see that the biorefinery investor gains 80% of the supply chain profit by leveraging its leader position.

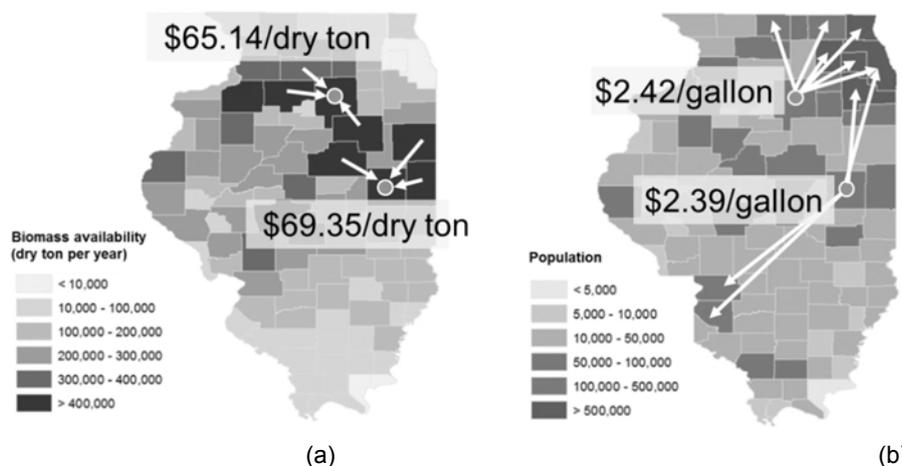


Figure 3. Optimal supply chain structure: (a) transportation of biomass feedstock from farmers to biorefineries with biomass availability as the map background; (b) transportation of biofuel product from biorefineries to consumers with population density as the map background.

At this optimal solution, the cost for producing one gallon of fuel ethanol is \$1.91. Capital investment accounts for the largest portion of the fuel ethanol cost, equalling 41%. The second largest component is the biomass harvesting cost, which accounts for 29% of the fuel ethanol cost. The fixed and variable O&M costs together share 8% of the fuel ethanol cost. The transportation of biomass also accounts for a significant portion (18%) of the fuel ethanol cost, because of the lower energy density of biomass. Since the energy density of fuel ethanol is significantly improved, the transportation cost of biofuel accounts for 4% of the fuel ethanol cost.

To compare the computational performance of the proposed successive piecewise approximation algorithm with that of the direct solution using state-of-the-art global optimizer, BARON 12, we discuss the model statistics and computational results of both methods below. The single-level MINLP problem involves 10 discrete variables, 285 continuous variables, and 362 constraints. We solve it directly using BARON 12 and it fails to converge after 20 hours. The relative gap at the time when it was terminated is 67.9%. In contrast, the successive piecewise approximation algorithm converges to the global optimal solution in about 8.6 hours. The relative gap is less than 0.1%. The algorithm takes a total of 7 iterations. As the algorithm proceeds, the numbers of variables and constraints increase. The MILP piecewise approximation in the first iteration involves 140 discrete variables, 445 continuous and SOS1 variables, and 712 constraints, while the MILP piecewise approximation in the 7<sup>th</sup> iteration involves 140 discrete variables, 875 continuous and SOS1 variables, and 867 constraints. Therefore, it is shown that the successive piecewise approximation algorithm is much more efficient in solving the reformulated MINLP problem considered in this work.

## 6. Conclusions

A novel game-theoretic modelling and optimization framework was proposed for the design and strategic planning of non-cooperative biofuel supply chains. We formulated a bilevel MINLP problem to model the leader-follower relationship and competition among the followers under the assumption of the single-leader-

multiple-follower Stackelberg game and the generalized Nash equilibrium. The upper level problem was a nonconvex MINLP, and the lower level problems are LPs. Applications of the proposed framework were demonstrated via a case study. We observed that the biofuel company gains most of the profit of the entire supply chain by leveraging the leader position. On the other hand, the computational experiments showed that the proposed solution strategy could improve the solution efficiency by at least an order of magnitude.

## References

- Akgul, O., Shah, N., Papageorgiou, L. G., 2012, Economic optimisation of a UK advanced biofuel supply chain. *Biomass and Bioenergy*, 41, 57-72.
- Bai Y., Ouyang Y., Pang J.S., 2012, Biofuel supply chain design under competitive agricultural land use and feedstock market equilibrium, *Energy Economics*, 34(5), 1623-1633.
- Bard J.F., 1998, *Practical bilevel optimization: algorithms and applications*, Kluwer Academic Publishers, Dordrecht, Netherlands.
- Bergamini M.L., Grossmann I., Scenna N., Aguirre P., 2008, An improved piecewise outer-approximation algorithm for the global optimization of MINLP models involving concave and bilinear terms, *Computers & Chemical Engineering*, 32(3), 477-493.
- Facchinei F., Kanzow C., 2007, Generalized Nash equilibrium problems, *4OR*, 5(3), 173-210.
- Garcia, D.J., You, F., 2015, Multiobjective optimization of product and process networks: General modeling framework, efficient global optimization algorithm, and case studies on bioconversion. *AIChE Journal*, 61(2), 530-554.
- Gebreslassie, B.H., Slivinsky, M., Wang, B., You, F., 2013, Life Cycle Optimization for Sustainable Design and Operations of Hydrocarbon Biorefinery via Fast Pyrolysis, Hydrotreating and Hydrocracking. *Computers & Chemical Engineering*, 50, 71-91.
- Gong, J., You, F., 2014, Global Optimization for Sustainable Design and Synthesis of Algae Processing Network for CO<sub>2</sub> Mitigation and Biofuel Production using Life Cycle Optimization. *AIChE Journal*, 60, 3195-3210.
- Gong, J., You, F., 2015, Value-Added Chemicals from Microalgae: Greener, More Economical, or Both? *ACS Sustainable Chemistry & Engineering*, 3, 82-96.
- Hasan M., Karimi I., 2010, Piecewise linear relaxation of bilinear programs using bivariate partitioning, *AIChE Journal*, 56(7), 1880-1893.
- Padberg M., 2000, Approximating separable nonlinear functions via mixed zero-one programs, *Operations Research Letters*, 27(1), 1-5.
- Ryu J.H., Dua V., Pistikopoulos E.N., 2004, A bilevel programming framework for enterprise-wide process networks under uncertainty, *Computers & Chemical Engineering*, 28(6-7), 1121-1129.
- Sharma, P., Romagnoli, J.A., 2011, Strategic decision analysis of multi-product biorefineries. *Chemical Engineering Transactions*, 25.
- Tong, K., You, F., Rong, G., 2014, Robust design and operations of hydrocarbon biofuel supply chain integrating with existing petroleum refineries considering unit cost objective. *Computers & Chemical Engineering*, 68, 128-139.
- Von Stackelberg H., Bazin D., Hill R., Urch L., 2011, *Market structure and equilibrium*, Springer, Berlin, Germany.
- Wang, B., Gebreslassie, B.H., You, F., 2013, Sustainable Design and Synthesis of Hydrocarbon Biorefinery via Gasification Pathway: Integrated Life Cycle Assessment and Technoeconomic Analysis with Multiobjective Superstructure Optimization. *Computers & Chemical Engineering*, 52, 55-76.
- Yeh K., Lee J.H., Whittaker C., Realf M.J., Two Stage Bilevel Programming Approach for Representation of Biorefinery Investment Decision Making in a Pre-Established Timberlands Supply Chain, 8th International Conference on Foundations of Computer-Aided Process Design, Cle Elum, Washington, USA.
- You F., Grossmann I.E., 2011, Stochastic inventory management for tactical process planning under uncertainties: MINLP models and algorithms, *AIChE Journal*, 57(5), 1250-1277.
- You F., Tao L., Graziano D.J., Snyder S.W., 2012, Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input-output analysis, *AIChE Journal*, 58(4), 1157-1180.
- You F., Wang B., 2011, Life Cycle Optimization of Biomass-to-Liquid Supply Chains with Distributed-Centralized Processing Networks, *Industrial & Engineering Chemistry Research*, 50(17), 10102-10127.
- Yue, D., Kim, M.A., You, F., 2013, Design of Sustainable Product Systems and Supply Chains with Life Cycle Optimization Based on Functional Unit: General Modeling Framework, Mixed-Integer Nonlinear Programming Algorithms and Case Study on Hydrocarbon Biofuels. *ACS Sustainable Chemistry & Engineering*, 1, 1003-1014.
- Yue, D., You, F., 2014, Fair Profit Allocation in Supply Chain Optimization with Transfer Price and Revenue Sharing: MINLP Model and Algorithm for Cellulosic Biofuel Supply Chains. *AIChE Journal*, 60, 3211-3229.
- Yue D., You F., Snyder S.W., 2014, Biomass-to-bioenergy and biofuel supply chain optimization: Overview, key issues and challenges, *Computers & Chemical Engineering*, 66, 36-56.