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Investment analysis of a research and development project for cellulosic ethanol production in Brazil

Reynaldo L. N. Taylor–de–Lima[1,2,*], Luiz Fernando L. Legey[2], Luiz Fernando M. Bandeira[3] and Adriano Fraga[3]

[1]*TL CONSULTORIA, Taylor de Lima Consultoria Ltda ME, Rua Viúva Lacerda, 249, Humaitá, 22261–050 Rio de Janeiro, RJ, Brazil.*

[2]*Department of Energy Planning, Graduate School of Engineering (COPPE), The Federal University of Rio de Janeiro (UFRJ), Centro de Tecnologia, Bloco C, Sala 211, Cidade Universitária, Ilha do Fundão, 21941–972 Rio de Janeiro, RJ, Brazil.*

[3]*Petrobras Research Centre – Avenida Horácio Macedo, 950, Cidade Universitária, Ilha do Fundão, Rio de Janeiro, RJ – 21941–915, Brazil.*

Abstract

This paper analyses the decision–making process of investments in research and development (R&D) projects. A case–study of the development of a technology based on the biochemical conversion of sugarcane bagasse for the production of lignocellulosic ethanol in Brazil is presented. The methodology used is based on the representation of development stages and decision gates, which together with decision trees is able to handle the many uncertainties related to R&D projects. In each decision gate, three possible options are simulated: abandoning the project (i.e., ceasing investments), maintaining its course, or improving its performance by adding more resources. This allows for a wait–and–see approach that incorporates identified sources of uncertainty at intermediate stages of development, thus increasing the chances of project feasibility. Comparisons of project values with and without flexibility — i.e., when options are available or not — show that while the project's value without flexibility is negative, it becomes positive when flexibility exists.

Keywords: *biomass conversion; cellulosic ethanol; research and development; economic feasibility; decision analysis; uncertainty.*

Nomenclature

X	conversion yield (litres of ethanol / dry ton of biomass)
V	project value (US$ million)
$E[V]$	expected value of V
p	transition probability for the optimistic scenario of technological performance
q	transition probability for the intermediate scenario of technological performance
r_t	discount rate in the interval $(t, t+1]$ (%)
$c(t)$	investment at instant t for the continue option (US$ million)
$a(t)$	additional investment at instant t for the improve option (US$ million)
M	high extreme value achieved for $V_T(X_T)$
m	low extreme value achieved for $V_T(X_T)$

Subscripts / Superscripts

t	time t
T	time of the project's conclusion
C	continue option
M	improve option
opt	optimistic scenario of technological uncertainty
int	intermediate scenario of technological uncertainty
pes	pessimistic scenario of technological uncertainty

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[*] Corresponding author

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1. Introduction

Biofuels represent an important alternative to mitigate the effects of climate change and crude oil depletion. Second–generation biofuels can be produced from biomass, in particular from lignocellulosic materials, such as agricultural waste [1]. Typically, their composition is as follows: 40% to 50% cellulose, 25% to 30% hemicellulose, 15% to 20% lignin and traces of pectin, nitrogenous and inorganic compounds [2]. They are considered interesting raw materials because they are abundant and do not compete with food production. The challenge, however, is to prove that second–generation biofuels production can be economically feasible.

In order to assess the economic feasibility of different conversion processes for various types of biomass, several studies have proposed innovative production strategies as well as methodologies. Humbird et al. [3] describe in detail one potential biochemical ethanol conversion process, conceptually based upon core conversion and process integration research at the National Renewable Energy Laboratory (NREL) of the U.S. Department of Energy. The biochemical process presented by them converts corn stover into cellulosic ethanol by dilute–acid pretreatment, enzymatic saccharification, and co–fermentation. Also included is a detailed process design for an idealized production plant with equipment specification and dimensioning, capital expenditures estimation, input and utility consumption computation, and a techno–economic assessment of the process. Junqueira et al. [4] estimated economic and environmental impacts of sugarcane biorefineries in Brazil, considering improvements of industrial processes and biomass production systems, as well as technological assumptions and scenarios based on companies involved in the lignocellulosic ethanol production. Klein et al. [5] presented a techno–economic and environmental assessment of renewable jet fuel production in integrated Brazilian sugarcane biorefineries. Their assessment of biorefineries for producing renewable jet fuel was based either on hydroprocessed esters and fatty acids or hydrocarbons obtained by Fischer–Tropsch synthesis, and their conclusion was that all conversion technologies studied had climate change impact reduction of more than 70% when compared with fossil jet fuel.

Hernández et al. [6], Wan et al. [7], Wan et al. [8], Stoklosa et al. [9], Taylor–de–Lima et al. [10], Arora et al. [11], Longati et al. [12 and Mandegari et al. [13] present assessments of the techno–economic viability of biorefineries for different possible scenarios, but only for existing technological developments, with no discussion of the several research and development stages, in which investment decisions are subject to uncertainties, such as expected costs and performance considerations.

Nevertheless, there are studies that examine this topic. Huchzermeier and Loch [14] use the real options approach to evaluate flexibility and management of R&D projects under risk. In addition to the familiar real option of abandonment, they introduce a corrective action option that can be used along the project's development. In their real options model, not only market payoff is under uncertainty, but also operational variables — such as budget, product performance requirements, and schedule — are uncertain. Santiago and Vakili [15], followed the same approach as Huchzermeier and Loch, but considered how the increase in uncertainty and volatility impact overall project values, as well as the value of management flexibility in R&D projects. Subsequent papers attempted to generalize the settings introduced by these authors, as for example, the effects of a competitive market environment and the degree of innovation (Kettunen et al. [16] and procedures directed to R&D managers behaviour (Wang and Yang [17], Wang et al. [18]).

Other studies introduced other aspects involving the development of R&D projects. Koussis, Martzoukos, and Trigeorgis [19] examine issues such as optimal timing of R&D, the impact of lags in the realization of the R&D outcome, and the choice between accelerated versus sequential R&D. These authors show that such controls introduce path–dependency in the valuation of R&D projects and are costly, besides having an uncertain outcome, although with a value–enhancing expectation.

Wu et al. [20] and Pendharkar [21] discuss how interdependencies across R&D stages can be treated operationally in lattice–based valuation algorithms or via multistage stochastic integer programming. Context–specific contributions in R&D and technological development, with case studies on specific industries are presented in d'Halluin — for wireless network investments in cellular phone services —, in Forsyth, and Vetzal [22] and Khansa and Liginlal [23] — for information security, and in Pennings and Sereno [24] — for pharmaceutical R&D.

The difficulty with the studies in decision analysis and real options modelling for R&D projects development is that the complexity introduced into the models requires the adoption of simple binomial lattices or simple symmetric decision trees, to implement all model's features. In other words, complex settings are frequently unsuitable to model actual R&D projects.

More recently, Valdívia et al. [25] presented a decision analysis valuation model for use across a variety of capital intensive and medium to long term R&D projects. They provide a study case of a project focused on the production of cellulosic ethanol from municipal solid waste (MSW). The authors claim that their model proposes a flexible valuation methodology based on decision analysis, Net Present Value computations and Monte Carlo simulation, together with a user–friendly interface that — when used from the project's very initial phases until its completion — enables decision–makers to define realistic and productive targets throughout the full R&D project period. However, Valdivia et al. [25] consider no more than a few static scenarios for ethanol price forecasting, as well as for the rate that municipalities would be charged per ton of MSW treated, which greatly limits the market uncertainties considered. In addition, they do not develop a decision tree, as considered in several of the references mentioned before (e.g., Huchzermeier and Loch [14]; Santiago and Vakili [15]). This prevents them from following the evolution of a particular R&D project over time, and thus taking as acceptable unfavourable trajectories to the project's continuation.

Biorefineries for lignocellulosic ethanol production through biochemical route involve the following stages, each presenting specific technological challenges: 1. Pre–treatment (removal of lignin or hemicellulose, making cellulose more accessible to enzyme action); 2. Hydrolysis of carbohydrate polymers (free sugars production through enzymatic action); 3. Fermentation of hexoses and pentoses (ethanol production); 4. Distillation of the wine containing ethanol (Batalha et al, [26]).

The development of chemical processes is often divided into sequential phases, which demand larger investments as the scale is increased (Edwards, [27]). In lignocellulosic ethanol production, these phases are microscale, bench scale, pilot scale and demonstration scale. In each of them, process characteristics should be well understood so that good estimates of performance levels can be used in decision–making models.

Development begins on a microscale with small volume reactors (typically ml), high purity reagents, purified raw materials, conditions close to ideal for mass and heat transfer, as well as large number of experiments to improve process yields. In the bench scale, high purity raw materials and inputs are still used, together with particle size control. Studies are carried out to obtain conversion and kinetics data, more accurate mass balances and better product characterization (Harmsen [28]).

Table 1. Second–Generation Ethanol Commercial Plants with Biochemical Route.

SECOND-GENERATION CELLULOSIC ETHANOL COMERCIAL PLANTS WITH BIOCHEMICAL ROUTE			
Company	**Plant Location**	**Annual Capacity**	**Status**
Abengoa Bioenergy Biomass of Kansas	Hugoton, Kansas, USA	25 millions of gallons	Cellulosic ethanol production facility, commercially opened in October 2014, was purchased by Synata Bio Inc. in 2016.
Beta Renewables	Crescentino, Italy	20 millions of gallons	Cellulosic refinery, which was the world's first commercial-scale refinery, was shut down in 2017. It was acquired in 2018 by Versalis (ENI) and will be re-started until June, 2020.
DowDuPont	Nevada, Iowa, USA	30 millions of gallons	Operation disrupted in 2017. In 2018, it was bought by Verbio to produce renewable natural gas (RNG), with start by summer 2020.
Enviral	Leopoldov, Slovakia	15 millions of gallons	2G plant to be integrated into the existing 1G facilities at Leopoldov site. License agreement with Clariant for the Sunliquid technology. Plant in engineering project phase.
POET-DSM	Iowa, USA	25 millions of gallons	After initial difficulties with the Andritz system, POET announced pretreatment reactor redesign and implementation of on-site enzyme production. The 2G ethanol production was paused again in November, 2019.
Granbio	São Miguel dos Campos, Alagoas, Brazil	21 millions of gallons	Ethanol plant in operation since 2014. Difficulties with original technology led to plant modifications. Since 2017, ethanol production has been interrupted and shifted to cogeneration and electricity commercialization.
Omega Energy	Location to be defined in the sugarcane belt, USA	10 -15 millions of gallons	Omega Energy and Lasuca Sugar are currently completing necessary formalities for the 2G ethanol project with Praj `s "enfinity" technology.
Raízen	São Paulo, Brazil	11 millions of gallons	Plant is running and produced 4.35 millions of gallons of 2G ethanol in 2019.

[1] Sources: Voorhis (2016) [40] for Abengoa; Eni Press Release (February 8, 2020) [42] for Beta Renewables; Verbio Press Release (November 11, 2018) [48] for DowDuPont; Rarbach, M. (2020) [47] for Enviral; Kennedy (2017) [44] and Bioenergy International [41] for POET–DSM; Scaramuzzo & Agostini (2017) [46] for Granbio; Sapp, M. (2019) [45] for Omega Energy; and Raízen (2019) [48] for Raízen.

The pilot scale stage is characterised by the following features: 1. Preliminary transition from batch reactors to continuous process reactors; 2. Use of steam in energy transfers, instead of electric heating; 3. Less purification of enzymatic processes cocktails; 4. Better energy efficiencies through reductions in steam consumption; 5. Better use of energy in impellers and screws; 6. Greater concentrations in streams of products and intermediate compounds, so as to reduce equipment size and save energy for diluents removal. The equipment used should be scalable to the demonstrations stage. Difficulties in scaling–up equipment with moving parts that process solid streams and less sterilized conditions should impact biomass conversion yields. The process approaches commercial scale operating conditions, which causes a reduction in ethanol yields.

In the demonstration stage, flowcharts of equipment and processes should resemble those of commercial stage. This is especially relevant for processes with manipulation of solids, which present higher risks during scaling up. Raw materials must be at a purity level that makes their use feasible. All process must be interconnected and have compatible scales. Redundancies and intermediate storage should be optimized to reduce investments during the demonstration stage. Again, yield reductions are expected.

Since 2014, the technology for lignocellulosic ethanol production is being tested in different countries on a commercial scale. Table 1 shows the companies which has been leading the field. Although in operation, their plants had problems that still need to be addressed. Some of these problems are: (i) difficulties in biomass feeding and erosion in the pre–treatment reactor; (ii) diverse ethanol yields as a result of different operational possibilities, including different biomass types, enzyme cocktail compositions and fermentation microorganisms (Junqueira et al. [4]). Such technological variability and the resulting uncertainty make economic feasibility studies all the more relevant to indicate more promising alternatives.

This paper aims at contributing to the methodology of economic feasibility assessment under uncertainty conditions, by analysing investment decisions in a research and development (R&D) project for lignocellulosic ethanol production technology, specifically adapted to sugarcane bagasse conversion. It builds upon Humbird et al. [3], who studied a biochemical process for ethanol production, using corn stover as raw material, enzymatic hydrolysis with in–situ produced cellulase enzymes and co–fermentation with the bacteria *Zymomonas mobilis*, which simultaneously ferment C5 and C6 sugars. This process is capable of producing 231 millions of litres of cellulosic ethanol per year (61 millions of gallons per year), in a plant processing 2,000 metric tons of dry biomass per day (*ibid*.).

It is a common practice in the biofuels industry to ignore the value of any embedded managerial flexibilities in R&D projects [3, 4, 5, 25]. This occurs because the main valuation method generally used by research laboratories to assess a project’s value is the discounted cash flow (DCF) method, which does not capture the value of flexibility. This article presents a multistage investment decision model built via a complex asymmetric and unstructured decision tree that takes into account uncertainty in both technology development and market payoff. The market payoff is calculated through a mean reverting stochastic process — to model future ethanol prices — and Monte Carlo simulation. The main contribution of this model is to track the actual development process of the technology — as observed in laboratory and pilot plant — and to provide a comprehensive quantitative answer to the R&D investment decision analysis of a lignocellulosic ethanol production technology.

Finally, it should be mentioned that although the primary technology studied here is related to hydrous ethanol production, the feasibility analysis presented below incorporates a dehydration phase to produce anhydrous ethanol. The reason for that is the existence of a well–established international market for the use of the latter as a gasoline additive.

The paper is organized in four sections, besides this Introduction. Next section presents the methodology used in the economic feasibility analysis. Section 3 describes the application of this methodology to assess a R&D project for ethanol production and section 4 studies the payoff of the cellulosic ethanol production for different values of the technology`s yield. Section 5 discusses results and their implications and, finally, section 6 presents the conclusions of the study.

2. A model for economic assessment of a research and development project

Uncertainties play an important role in the value of R&D projects. Indeed, the project`s final technological performance may not correspond to initial expectations, development costs may turn out to be much higher than at first envisaged, delays may occur and market requirements related to product`s quality may affect the payoff of the project (Huchzermeier & Loch [14]). In addition, uncertainties may impact the project`s managerial flexibility value, i.e., the difference between its value when actively or passively managed, or yet when flexibilities are used as leverage to the project's development (Santiago & Vakili [15]). In other words, the practice of active management may lead to the project's economic feasibility (*ibid*, *ibid*).

Figure 1 presents a scheme of how the methodology of development stages and decision gates works. At each decision gate, technological development conditions are re–evaluated. It thus consists of a fairly simple multistage model that can provide comprehensive quantitative assessments and allows for the treatment of different sources of uncertainty. The present study builds upon the approach to decision analysis, as described in Anderson et al. [29] and Luenberger [30], and takes into account the works by Huchzermeier and Loch [14], Santiago and Vakili [15], Leite et al. [31], Crama et al. [32], and Stonebraker [33].

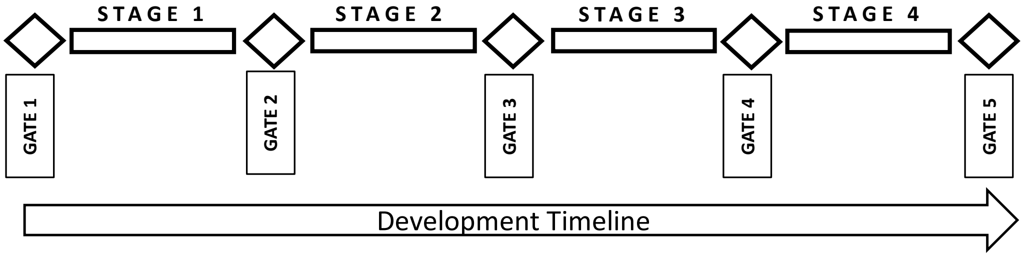


Figure 1. Development Stages and Decision Gates Methodology.

At each gate, an assessment of possible technological developments in next stage is made, taking into account uncertainty sources that can affect performance, here represented by the conversion process performance X. Thus, when a yield X_t is reached at the decision gate at time t, the yield X_{t+1} to be reached at the next gate, at time $t+1$, is uncertain. Incorporation of this uncertainty in a multi–stage model is made through a decision tree, as shown schematically in Figure 2. In this Figure, each node presents three possible courses of action: continue, improve (increase investment) or abandon the project.

A decision tree is characterised by, two types of nodes: decision nodes, in which the decision maker chooses one of the possible courses of action, and uncertainty nodes, where likely scenarios are assigned to a (subjective) probability (Anderson et al., [29]). For the model represented in Figure 2, there is a combination of these two node types, as shown in Figure 3, which details each node of Figure 2.

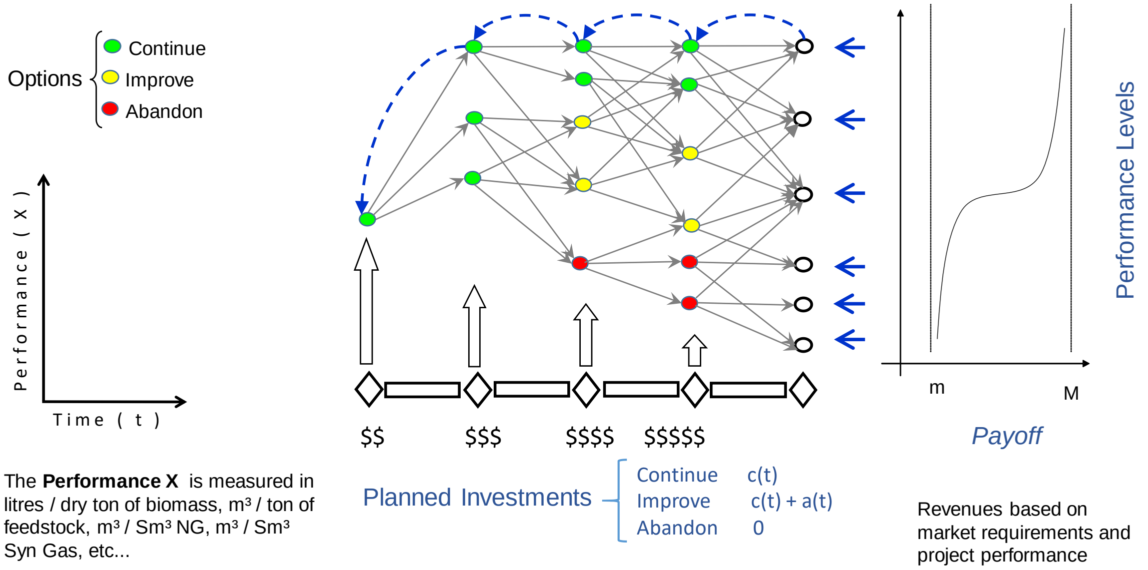


Figure 2. Multi–stage Model – Decision Tree Representation.

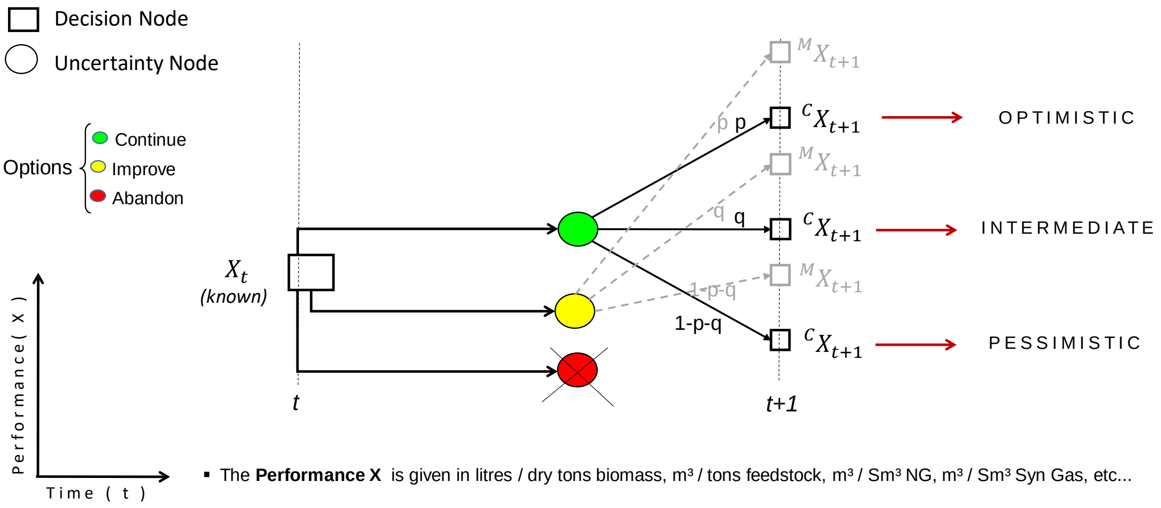


Figure 3. Decision Tree – Representation of One Node.

Equations (1) and (2) below show how the model calculates the values of the project at time t for the current yield X_t, or $V_t(X_t)$. Thus $^{C}V_t(X_t)$ is the value for the continue option and $^{M}V_t(X_t)$ is the value for the improve option. Further, $E\left[V_{t+1}\left(^{C}X_{t+1}\right)\right]$ and $E\left[V_{t+1}\left(^{M}X_{t+1}\right)\right]$represent, respectively, the expected project values of $V_{t+1}(X_{t+1})$ for the continue and improve options. In addition, $c(t)$ indicates the investment to be made at instant t for the continue option, while $a(t)$ represents the additional investment — i.e. to be added to $c(t)$ — at instant t , to improve technological performance, and r_t is the discount rate in the interval $(t\,,t+1]$.

$$^{C}V_t(X_t) = -c(t) + \frac{1}{1+r_t}E\left[V_{t+1}\left(^{C}X_{t+1}\right)\right] \tag{1}$$

$$^{M}V_t(X_t) = -\,c(t) - a(t) + \frac{1}{1+r_t}E\left[V_{t+1}\left(^{M}X_{t+1}\right)\right] \tag{2}$$

The expected values are computed through the following equations:

$$E\left[V_{t+1}\left({}^{C}X_{t+1}\right)\right] = p\, V_{t+1}\left({}^{C}X_{t+1}^{opt}\right) + qV_{t+1}\left({}^{C}X_{t+1}^{int}\right) + (1-p-q)V_{t+1}\left({}^{C}X_{t+1}^{pes}\right) \tag{3}$$

$$E\left[V_{t+1}\left({}^{M}X_{t+1}\right)\right] = pV_{t+1}\left({}^{M}X_{t+1}^{opt}\right) + qV_{t+1}\left({}^{M}X_{t+1}^{int}\right) + (1-p-q)V_{t+1}\left({}^{M}X_{t+1}^{pes}\right) \tag{4}$$

where ${}^{i}X_{t+1}^{j}$, $i = C, M$ and $j = opt,\ int, pes$, represent, as Figure 3 shows, the technological uncertainty related to process yield X_{t+1} in three possible scenarios: optimistic (*opt*), intermediate (*int*) and pessimistic (*pes*), with assigned (subjective) probabilities of, respectively, p , q and $1-p-q$, also called transition probabilities of technological performance.

The choice of the best alternative is guided by the following rules:

1. If ${}^{C}V_t(X_t) \geq 0$ and ${}^{C}V_t(X_t) \geq {}^{M}V_t(X_t)$, then choose continue and make
$$V_t(X_t) = {}^{C}V_t(X_t); \tag{5.a}$$
2. If ${}^{M}V_t(X_t) \geq 0$ and ${}^{M}V_t(X_t) \geq {}^{C}V_t(X_t)$, then choose improve and make
$$V_t(X_t) = {}^{M}V_t(X_t); \tag{5.b}$$
3. If ${}^{C}V_t(X_t) < 0$ and ${}^{M}V_t(X_t) < 0$, then choose abandon and make
$$V_t(X_t) = 0. \tag{5.c}$$

Equations (1) – (4) and rules (5) configures a backward recursive dynamic programming algorithm that can compute all node values $V_t(X_t)$ of the decision tree depicted in Figure 2. However, to apply the algorithm, it is necessary to know the values $V_T(X_T)$ at the time T of the project's conclusion or the date of the launching of the technology to the market. In some situations, this value $V_T(X_T)$ — known as the payoff of the technology developed — is directly affected by the market expectations on the performance of the specific product developed. For Santiago and Vakili [15] — and also for Huchzermeier and Loch [14] — the market payoff is assumed to achieve, in regular cases, a basic value that can easily be obtained, but in some special cases it is possible to achieve a premium payoff when the product's performance exceeds an uncertain market requirement.

However, in the case studied in this article, the product to be commercialized — cellulosic ethanol — is a commodity that must meet the same specifications as regular ethanol. Thus the payoff variability depends only on the performance of the process technology developed. Hence, the value $V_T(X_T)$ of the payoff of the technology developed in the R&D project is the Net Present Value (NPV) of a production plant designed for the performance level expressed by X_T. It would be desirable to have a continuous payoff curve for $V_T(X_T)$. Unfortunately, this is impractical as it would require innumerable conceptual engineering projects — and their associated capital investments and operating costs — to make a good estimate of the NPV of the production plant.

To cope with this issue, we will make use of two extreme values for $V_T(X_T)$, one defined as high, achieving the value $V_T(X_T) = M$, and another named low, for which $V_T(X_T) = m$. Intermediate values will then be interpolated by means of a generalized logistic curve, defined by the Equation

$$V_T\,(X_T) = m + \frac{M-m}{\left(C + Q\, e^{-a\left(X_T - X_{T_0}\right)}\right)^{1/b}} \tag{6}$$

Given M, m and X_{T_0}, the latter representing the value X_T for which $V_T(X_T) = 0$, the parameters C, Q, a and b will be estimated through Ordinary Least Squares (OLS).

It is important to observe that the reason for using a logistic curve is based on the fact that the chosen curve has to pass precisely through three points, as well as present a quasi–asymptotic behaviour at its extreme points, which suggests a change of concavity, and therefore an S format. Nevertheless, the choice is subjective and based on the authors' experience.

3. Economic assessment of cellulosic ethanol research and development

Figure 4 depicts a typical arrangement of development stages and decision gates for research and development of process technologies, in accordance to the sequential phases discussed in section 1 for the development of chemical processes. At gate 1, a decision on whether to begin developing the project is made, which if positive unfolds in subsequent stages named microscale, bench scale, pilot scale and demonstration scale. In general, each stage takes, respectively, two years, one year, three years and two years to complete. When the yield in the last stage is below expectations, additional investments to improve plant performance are often considered and evaluated in further demonstration stages. The case study presented here stipulates three demonstration stages (A, B and C), the first one lasting for two years and the latter two for one and a half years each.

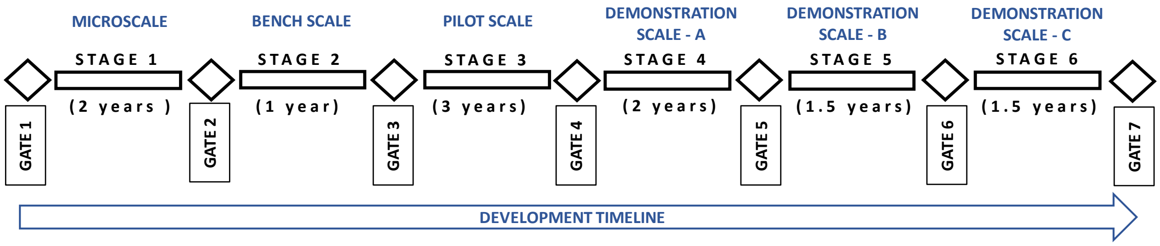


Figure 4. Development Stages and Decision Gates – Lignocellulosic Ethanol.

The maximum theoretical yield of the conversion process is 434.0 litres of ethanol per dry ton of bagasse, with 273.0 litres per dry ton coming from six–carbon (C6) sugars and 161.0 litres per ton from C5 sugars. In commercial scale, the conversion yields to ethanol reported by the companies with plants in operation (see Table 1) vary widely on account of different operational strategies. Clariant Group Biotechnology, licensor of the process used by Enviral, achieves up to 300 litres of ethanol / dry ton of sugar cane bagasse [34]. Atlantic Consulting, adopting an integrated enzyme production scheme, achieves 286 litres / dry ton of biomass [35]. POET–DSM, at its Iowa plant, achieves 265 litres / dry ton of corn stover, with the goal of reaching 275 litres / dry ton of biomass [36]. Praj reports that its enfinity technology leads to a conversion of 325–327 litres / dry ton of corn cobs, as well as to 260–290 litres / dry ton of sugarcane bagasse [37]. Finally, Raízen began with 91 litres / dry ton of sugarcane bagasse, in 2015, improved to 211 litres / dry ton of sugarcane bagasse, in 2016, and aims to reach 289 litres of ethanol / dry ton of biomass in the near future [38].

Assuming an overall efficiency of 76%, a maximum conversion of 330.0 litres per dry ton of sugarcane bagasse (or 390.0 litres per dry ton of bagasse ground fibre) is adopted (Humbird et al., 2011 [3]). As a lower bound to the conversion efficiency we assumed an ethanol yield of around 85.0 litres per dry ton of sugarcane bagasse (or 100 litres per dry ton of bagasse ground fibre), coming mainly from C6 sugars, which corresponds to the initial conversion reported by Raízen in 2015.

Table 2. Research and Development Project – Scheduled Investments and Expected Yields.

"Microscale"	"Bench Scale"	"Pilot Scale"	"Demonstration A"	"Demonstration B"	"Demonstration C"
Stage 1 (2 years)	Stage 2 (1 year)	Stage 3 (3 years)	Stage 4 (2 years)	Stage 5 (1.5 years)	Stage 6 (1.5 years)

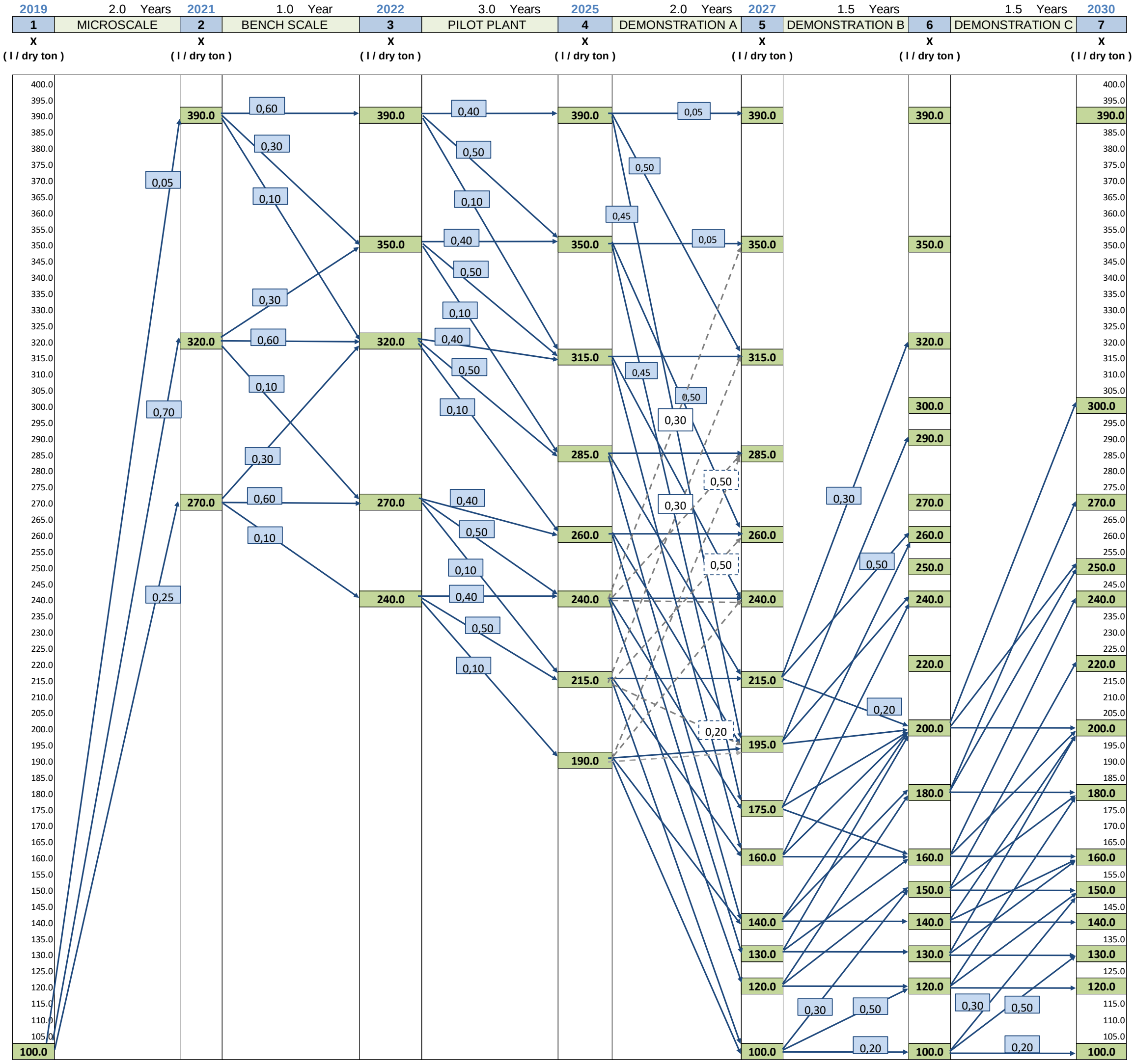
Investment (MM US$)	Investment (MM US$)	Investment (MM US$)	Investment (MM US$)	Investment (MM US$)	Investment (MM US$)
c (1) = 0.6	c (2) = 0.2	c (3) = 3.9	c (4) = 56.0	c (5) = 15.4	c (6) = 15.4
a (1) =	a (2) =	a (3) =	a (4) = 15.4	a (5) =	a (6) =

Discount Rate	3.63%	Discount Rate	3.63%	Discount Rate	3.63%	Discount Rate	3.63%	Discount Rate	3.63%	Discount Rate	3.63%
Adjusted Rate	7.39%	Adjusted Rate	3.63%	Adjusted Rate	11.29%	Adjusted Rate	7.39%	Adjusted Rate	5.49%	Adjusted Rate	5.49%

X_1	X_2	p, q, …	X_2	X_3	p, q, …	X_3	X_4	p, q, …	X_4	X_5	p, q, …	X_5	X_6	p, q, …	X_6	X_7	p, q, …
100.0	390.0	0.05	390.0	390.0	0.60	390.0	390.0	0.40	390.0	390.0	0.05	215.0	320.0	0.30	200.0	300.0	0.30
	320.0	0.70		350.0	0.30		350.0	0.50		315.0	0.50		260.0	0.50		250.0	0.50
	270.0	0.25		320.0	0.10		315.0	0.10		195.0	0.45		200.0	0.20		200.0	0.20
			320.0	350.0	0.30	350.0	350.0	0.40	350.0	350.0	0.05	195.0	290.0	0.30	180.0	270.0	0.30
				320.0	0.60		315.0	0.50		260.0	0.50		240.0	0.50		250.0	0.50
				270.0	0.10		285.0	0.10		175.0	0.45		200.0	0.20		180.0	0.20
			270.0	320.0	0.30	320.0	315.0	0.40	315.0	315.0	0.05	175.0	260.0	0.30	160.0	240.0	0.30
				270.0	0.60		285.0	0.50		240.0	0.50		200.0	0.50		200.0	0.50
				240.0	0.10		260.0	0.10		160.0	0.45		160.0	0.20		160.0	0.20
						270.0	260.0	0.40	285.0	285.0	0.05	160.0	240.0	0.30	150.0	220.0	0.30
							240.0	0.50		215.0	0.50		200.0	0.50		180.0	0.50
							215.0	0.10		140.0	0.45		160.0	0.20		150.0	0.20
						240.0	240.0	0.40	260.0	260.0	0.05	140.0	200.0	0.30	140.0	200.0	0.30
							215.0	0.50		195.0	0.50		180.0	0.50		180.0	0.50
							190.0	0.10		130.0	0.45		140.0	0.20		140.0	0.20
									240.0	240.0	0.05	130.0	200.0	0.30	130.0	200.0	0.30
										175.0	0.50		160.0	0.50		160.0	0.50
										120.0	0.45		130.0	0.20		130.0	0.20
									215.0	215.0	0.05	120.0	180.0	0.30	120.0	180.0	0.30
										160.0	0.50		150.0	0.50		150.0	0.50
										100.0	0.45		120.0	0.20		120.0	0.20
									190.0	190.0	0.05	100.0	150.0	0.30	100.0	150.0	0.30
										140.0	0.50		120.0	0.50		130.0	0.50
										100.0	0.45		100.0	0.20		100.0	0.20

The adopted yields for the conversion process over all development stages, X_{t+1} $(t = 1, \dots, 6)$, as well as the probabilities p, q and $1 - p - q$, and the investment terms $c(t)$ and $a(t)$, $(t = 1, \dots, 6)$, were estimated based on the experience of the two authors from the industry, who are directly enrolled in the R&D activities.

Table 2 and Figure 5 below show the estimates for X_{t+1} $(t = 1, \dots, 6)$, the yields for the conversion process over all development stages, along with estimates for probabilities p, q and $1 - p - q$, which correspond, respectively, to optimistic, intermediate and pessimistic scenarios1. These parameters are estimated according to the following rationale: (a) a significant expected improvement for X_{t+1} in the microscale stage, due to the large number of experiments carried out through the screening procedures of this stage; (b) the difficulty to maintain process yields on bench scale; and (c) the strong reductions in X_{t+1} yields expected on both pilot and demonstration scales.



The choice of a risk–free annual discount rate for Brazil is a matter of great discussions among economists and investors. Here we decided to use the real (inflation free) interest of medium term (2026) Brazilian Treasure Bond (**http://www.tesouro.fazenda.gov.br/tesouro–direto–precos–e–taxas–dos–titulos**, accessed 31.03.2020).

Figure 5. Decision Tree – Lignocellulosic Ethanol.

In terms of investment needs, $c(t)$ indicates the outlay at time t for the option continue the project and $a(t)$ represents the additional investment to be made on top of $c(t)$ at time t, in order to improve technological performance. Table 2 shows the estimates of $c(t)$ and $a(t)$ for the six stages of development. In addition, it shows the discount rates r_t in each stage, corresponding to a risk–free annual discount rate of 3,63%.

It is important to mention that in Gates 5 and 6, development goes on only if the ethanol yield X_{t+1} obtained so far does not exceed the level of 240 $l/$ dry ton of sugarcane bagasse ground fibre, which is considered to make the technology acceptable from a commercial point of view. Thus, the decision to continue the development will focus only on cases for which $X_{t+1} \leq$ 240 $l/$ dry ton of sugarcane bagasse ground fibre, and when investments in adaptations of the demonstration plant are likely to improve performance. It is considered that such plant adaptations will take a full year, plus six months of additional tests. In Gate 7, a commercial plant will be built only if X_7 exceeds $240\ l/$ dry ton of sugarcane bagasse ground fibre.

4. Payoff of the Cellulosic Ethanol Technology

Each node of the decision tree in Figure 5 has three branches representing three scenarios (optimistic, intermediate and pessimistic) for ethanol yields in the next development stage, along with their respective probabilities. In a backward recurrence procedure, to determine $V_{t-1}(X_{t-1})$ at time $t-1$, it is necessary to know $V_t(X_t)$ at node t , beginning with $V_T(X_T)$ at time T, the date of the technology`s market launch.

As discussed in section 2, the payoff $V_T(X_T)$ is described by a generalized logistic function defined in equation (6). However, before proceeding with the estimation of this equation, M and m have to be computed, as they are NPVs of the project, when yields are high and costs are low (M), and when yields are low and costs are high (m). The remaining parameter X_{T_0}— the yield that barely compensates investments on a commercial plant (i.e., $V_T(X_T) = 0$) — is assumed to be 240 litres per dry ton of sugarcane bagasse ground fibre.

4.1 Payoff Values

The data used to determine payoff values is based on Humbird et al. [3], with adaptations made to Brazilian conditions along the lines of the procedure described by the senior authors in Taylor–de–Lima et al. [10] and provided in an electronic Supplementary Appendix. Table 3 shows the Cost Structure of a lignocellulosic ethanol commercial plant in US dollars (referred to the year 2019), in both high and low payoff settings. The Fixed Capital Investment in Brazil (FCI–BR) was obtained by adjusting the United States Gulf Coast (USGC) Fixed Capital Investment (FCI) of US$ 511,955,281 through an internalization factor of 1.7843 (Da Silva[38]), thus providing an estimated FCI–BR of US$ 913,481,808, for a typical commercial plant. According to the American Association of Cost Engineers – AACE [39], such an estimate can vary between –20% to +30% of its typical value. Therefore, the FCI–BR can be as low as US$ 730,785,466 or as high as US$ 1,187,526,350. Consequently, these figures were adopted in the computation of high and low payoff values, respectively.

As for the remaining cost items, estimations are based on the rationale that annual variable operating costs are identical for both payoff values, because the amount of inputs used in either case are equivalent, whereas annual fixed operating costs vary in conformity to established percentage rates, although the labour costs, which are part of the fixed operating costs, remain the same.

Project revenues computations are based on data adapted from the mass balance presented in Humbird et al. (*ibid.*), which discriminates technical coefficients for products, inputs and utilities. Table 4 shows the several revenue components, considering constant prices for products, inputs and utilities in US dollars referred to the year 2019. In terms of productivity yields, we considered an approximate yield of $X_T = 390\ l/$ dry ton of sugarcane bagasse ground fibre for the high payoff and a yield of $X_T = 100\ l/$ dry ton of sugarcane bagasse ground fibre for the low payoff.

Table 3. Lignocellulosic Ethanol Commercial Plant – Cost Structure.

LIGNOCELLULOSIC ETHANOL - BIOCHEMICAL ROUTE - COST STRUCTURE (US$)		
Cost Item	**High Payoff (M)**	**Low Payoff (m)**
Fixed Capital Investment (FCI-BR)	**730,785,446**	**1,187,526,350**
Annual Variable Operating Costs	**39,864,648**	**39,864,648**
Annual Fixed Operating Costs	**28,146,967**	**45,046,381**
Labour Costs	583,108	583,108
Other Fixed Costs	27,563,859	44,463,272
Benefits and general overhead (90% Labour Costs)	524,798	524,798
Materials - Maintenance (3.0% FCI-BR per year)	21,923,563	35,625,791
Insurance and taxes (0.7% FCI-BR per year)	5,115,498	8,312,684

Table 4. Lignocellulosic Ethanol Commercial Plant – Revenues.

LIGNOCELLULOSIC ETHANOL - BIOCHEMICAL ROUTE - REVENUES (US$)		
Revenue Item	**High Payoff (M)**	**Low Payoff (m)**
Annual Gross Revenue	**155,548,647**	**35,043,848**
Anhydrous ethanol	**150,158,879**	**29,654,081**
Quantity (litres)	231,013,660	59,308,161
Price (US$ / Litre)	0.650	0.500
Grid electricity	**5,050,737**	**5,050,737**
Quantity (kWh)	107,622,770	107,622,770
Price (US$ / kWh)	0.0469	0.0469
Area 100 electricity	**339,031**	**339,031**
Quantity (kWh)	7,224,190	7,224,190
Price (US$ / kWh)	0.0469	0.0469

Finally, to compute the payoff values, one considered an annual cash flow over 25 years, discounted at the minimum attractiveness rate of 9% per year, as recommended for projects with a sustainability bias. Table 5 depicts the computed deterministic average high and low payoff values, *M* and *m*, showing that the latter is negative (see the electronic Supplementary Appendix).

Table 5. High and low deterministic payoff values (US$ million).

LIGNOCELLULOSIC ETHANOL - DETERMINISTIC PAYOFF VALUES (US$ million)	
High Payoff Value (M)	**Low Payoff Value (m)**
128	**-1,031**

4.2 Stochastic Analysis

The analysis presented in this section aims at incorporating uncertainties that affect some variables which may have significant impact on the project’s payoff values. In this sense, biomass and ethanol prices are especially important and thus will be the subject of a stochastic analysis that follows the approach introduced by the senior authors in Taylor–de–Lima et al (*ibid*.).

In summary, this approach proceeds along the following steps:

(1) Assume the variables follow a stochastic process, such as the Mean Reverting Stochastic Process (MRP);
(2) Using historical data, estimate the parameters of the MRP model for each variable;
(3) Generate synthetic series through a Monte Carlo simulation procedure; and
(4) Compute NPVs for a chosen number of series of future prices.

Table 6 shows the results obtained from Monte Carlo simulations of 5,000 trajectories of sugarcane bagasse and anhydrous ethanol prices in a high payoff value setting (*M*), with a 30% increase (premium) in the price of ethanol. It shows, among other variables, the maximum, minimum and average values of the project`s NPV, as well as an indicator of when the NPV for a particular run is positive (1) or negative (0). Detailed results from the analysis can be found in the electronic Supplementary Appendix. Table 6 shows that simulations indicate a positive average NPV of US$ 416 million and that, from a total of 5,000 runs, there are 4,950 runs that present positive NPVs. This means that the estimated risk of a negative NPV is just 1.00 %. Figure 6 presents the NPV histogram of the simulated high payoff values.

Table 6. Monte Carlo Simulation – Summary of 5,000 Runs (High Payoff Setting, with Premium of 30% on Ethanol Prices).

Scenario	**DISCOUNTED CASH FLOW FOR EACH SIMULATION (MM US$)**								**Risk NPV<0** **1.00%**
Items	Gross Revenue	Fixed Cost	Variable Cost	Other Expenses	Taxes	Net Income	Fixed Capital Investment	NPV	**Scenarios NPV > 0**
Minimum	657	213	274	124	11	-224	603	-441	**4950**
Maximum	3,859	213	302	124	1,025	1,953	603	1,736	
Mean	1,864	213	289	124	347	633	603	416	
1	657	213	275	124	11	-224	603	-441	0
2	936	213	290	124	48	3	603	-215	0
3	1,498	213	290	124	225	387	603	170	1
4	1,595	213	288	124	255	457	603	240	1
5	2,234	213	285	124	473	881	603	664	1
51	1,514	213	288	124	227	404	603	187	1
52	1,796	213	287	124	323	590	603	373	1
53	1,460	213	288	124	212	364	603	147	1
54	1,407	213	291	124	190	331	603	114	1
55	2,114	213	286	124	432	801	603	584	1
56	2,249	213	283	124	479	892	603	675	1
57	2,271	213	286	124	485	905	603	688	1
4,996	1,899	213	283	124	361	660	603	443	1
4,997	1,343	213	285	124	187	276	603	59	1
4,998	1,939	213	287	124	372	685	603	468	1
4,999	1,232	213	283	124	137	217	603	0	0
5,000	770	213	274	124	29	-128	603	-345	0

Results for the simulation of low payoff values (*m*) are shown in Table 7. The average NPV is negative and has a value of US$ –1,290 million. All NPVs are negative, indicating an estimated 100% risk of a negative NPV. Figure 7 presents the NPV histogram of the simulated low payoff values.

Table 8 brings together the computed deterministic and stochastic average values for high and low payoff NPVs. From this Table, it is possible to see that the incorporation of the uncertainty in biomass and ethanol prices emphasises the differences between deterministic and stochastic values of *M* and *m*. Since the latter are more robust, they will be used in the estimation of the logistic function.

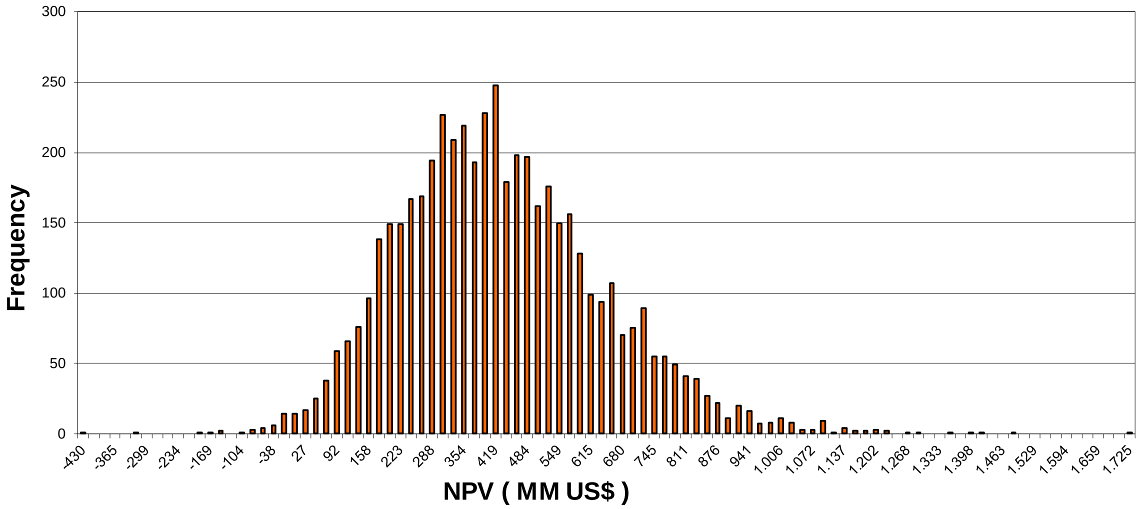


Figure 6. NPV Histogram for 5,000 runs (High Payoff Setting).

Table 7. Monte Carlo Simulation – Summary of 5,000 Runs (Low Payoff Setting).

Scenario	**DISCOUNTED CASH FLOW FOR EACH SIMULATION (MM US$)**								**Risk NPV<0** **100.0%**
Items	Gross Revenue	Fixed Cost	Variable Cost	Other Expenses	Taxes	Net Income	Fixed Capital Investment	NPV	**Scenarios NPV > 0**
Minimum	68	342	274	202	0	-1173	980	-1,496	**0**
Maximum	1,453	342	302	202	174	31	980	-301	
Mean	287	342	289	202	0	-964	980	-1,290	
1	68	342	275	202	0	-1168	980	-1,491	0
2	85	342	290	202	0	-1166	980	-1,490	0
3	166	342	290	202	0	-1086	980	-1,410	0
4	200	342	288	202	0	-1050	980	-1,375	0
5	450	342	285	202	0	-796	980	-1,124	0
51	191	342	288	202	0	-1059	980	-1,385	0
52	308	342	287	202	0	-941	980	-1,268	0
53	175	342	288	202	0	-1075	980	-1,400	0
54	156	342	291	202	0	-1097	980	-1,422	0
55	339	342	286	202	0	-908	980	-1,235	0
56	404	342	283	202	0	-841	980	-1,169	0
57	434	342	286	202	0	-813	980	-1,145	0
4,996	233	342	283	202	0	-1012	980	-1,336	0
4,997	136	342	285	202	0	-1110	980	-1,434	0
4,998	305	342	287	202	0	-944	980	-1,269	0
4,999	124	342	283	202	0	-1120	980	-1,444	0
5,000	68	342	274	202	0	-1167	980	-1,490	0

Table 8. Deterministic and Stochastic average payoff values (US$ million).

LIGNOCELLULOSIC ETHANOL - DETERMINISTIC AND STOCHASTIC PAYOFF VALUES (US$ million)		
	High Payoff Value (M)	**Low Payoff Value (m)**
Deterministic	**128**	**-1,031**
Stochastic	**416**	**-1,290**

4.3 Estimation of the Generalized Logistic Function

Parameters C, Q, a and b in equation 6 are estimated through Ordinary Least Squares (OLS), given $M = 416\ million$, $m = -1{,}290\ million$ and $X_{T_0} = 240l/dry\ \ ton$. Estimated values are presented in Table 9 and Figure 8 depicts the generalized logistic function incorporating these values.

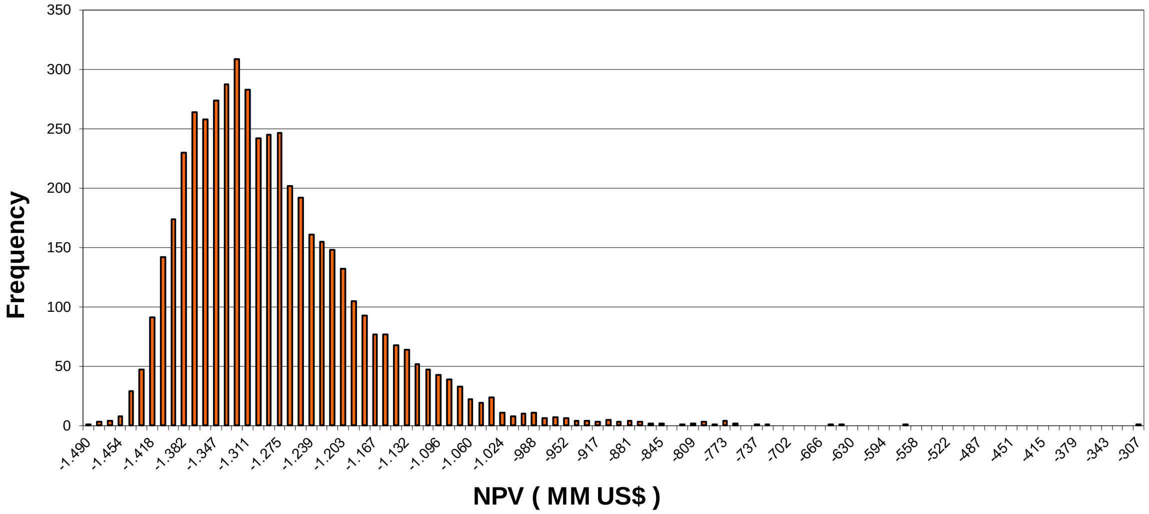


Figure 7. NPV Histogram for 5,000 runs (Low Payoff Setting).

Table 9. Generalized Logistic Function – OLS estimation.

GENERALIZED LOGISTIC FUNCTION
Estimated Parameters
C = 1.00000
Q = 0.32248
a = 0.02380
b = 0.14594

5. Results and discussion

Applying the methodology described in sections 2 and 3, as well as estimations presented in section 4, it is possible to build the decision trees shown in Figures 9 and 10. The decision tree in Figure 9 assumes that there will be no further improvement during Demonstration A stage, while the one in Figure 10 analyses the case where an attempt to improve yields is made during this stage.

Table 10. Results of the Decision Tree Analysis.

LIGNOCELLULOSIC ETHANOL - RESULTS OF THE DECISION TREE ANALYSIS	
Flexibility Options	**Project's Valuation (US$ millions)**
None	**- 110.0**
Continue or Abandon	**137.83**
Continue, Improve or Abandon	**166.39**

Overall results of the analysis are presented in Table 10, which shows two possible contexts of decision flexibility, one with the options of either to continue or to abandon the project, and another with three decision options: to continue, to improve or to abandon the R&D effort.

	X (l / dry ton)	$V_T (X_T)$ (MM US$)
6.0	400.0	416.0
5.8	395.0	416.0
5.6	**390.0**	**416.0**
5.4	385.0	416.0
5.2	380.0	416.0
5.0	375.0	416.0
4.8	370.0	416.0
4.6	365.0	416.0
4.4	360.0	416.0
4.2	355.0	416.0
4.0	**350.0**	**416.0**
3.8	345.0	416.0
3.6	340.0	416.0
3.4	335.0	416.0
3.2	330.0	416.0
3.0	325.0	416.0
2.8	**320.0**	**416.0**
2.6	315.0	416.0
2.4	310.0	416.0
2.2	305.0	416.0
2.0	**300.0**	**416.0**
1.8	295.0	415.9
1.6	290.0	415.8
1.4	285.0	415.6
1.2	280.0	415.2
1.0	275.0	414.2
0.8	**270.0**	**411.9**
0.6	265.0	406.7
0.4	260.0	395.2
0.2	255.0	369.6
0.0	**250.0**	**314.7**
-0.2	245.0	203.0
-0.4	**240.0**	**0.0**
-0.6	235.0	-303.2
-0.8	230.0	-645.5
-1.0	225.0	-928.7
-1.2	**220.0**	**-1,108.7**
-1.4	215.0	-1,204.7
-1.6	**210.0**	**-1,251.2**
-1.8	205.0	-1,272.6
-2.0	**200.0**	**-1,282.3**
-2.2	195.0	-1,286.6
-2.4	190.0	-1,288.5
-2.6	185.0	-1,289.3
-2.8	**180.0**	**-1,289.7**
-3.0	175.0	-1,289.9
-3.2	170.0	-1,289.9
-3.4	165.0	-1,290.0
-3.6	**160.0**	**-1,290.0**
-3.8	155.0	-1,290.0
-4.0	**150.0**	**-1,290.0**
-4.2	145.0	-1,290.0
-4.4	**140.0**	**-1,290.0**
-4.6	135.0	-1,290.0
-4.8	**130.0**	**-1,290.0**
-5.0	125.0	-1,290.0
-5.2	**120.0**	**-1,290.0**
-5.4	115.0	-1,290.0
-5.6	110.0	-1,290.0
-5.8	105.0	-1,290.0
-6.0	**100.0**	**-1,290.0**

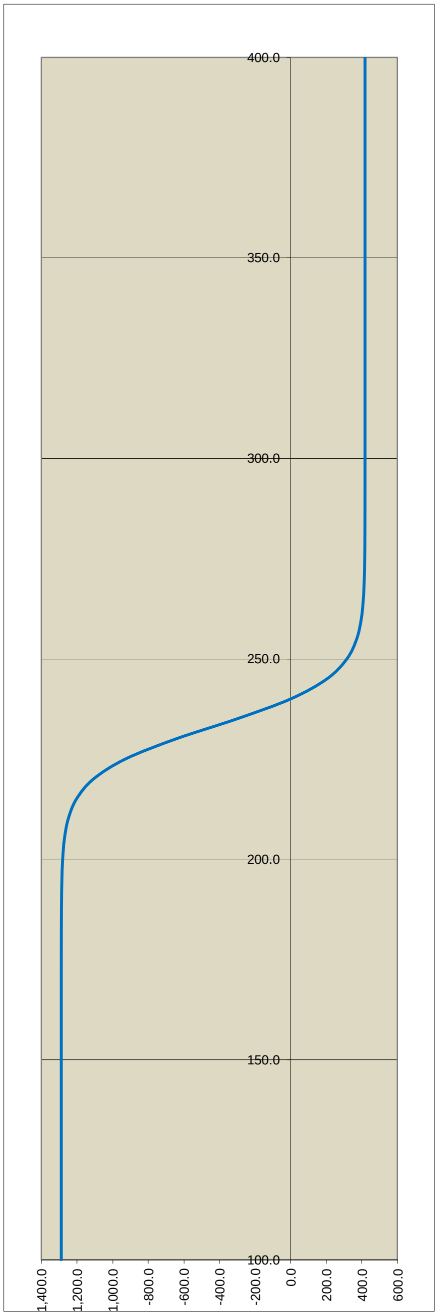


Figure 8. Generalised Logistic Function – Graphic Representation.

TEMPO DE DURAÇÃO DAS ETAPAS E TAXA DE DESCONTO AJUSTADA

ETAPA 1 (anos)	2.0	ETAPA 2 (anos)	1.0	ETAPA 3 (anos)	3.0	ETAPA 4 (anos)	2.0	ETAPA 5 (anos)	1.5	ETAPA 6 (anos)	1.5
Taxa Ajustada =	7.39%	Taxa Ajustada =	3.63%	Taxa Ajustada =	11.29%	Taxa Ajustada =	7.39%	Taxa Ajustada =	5.49%	Taxa Ajustada =	5.49%

INVESTIMENTO EM PESQUISA E DESENVOLVIMENTO

		INVESTIMENTO	I1	INVESTIMENTO	I2	INVESTIMENTO	I3	INVESTIMENTO	I4	INVESTIMENTO	I5	INVESTIMENTO	I6
Montante a investir para	CONTINUAR	c (t) =	0.6	c (t) =	0.2	c (t) =	3.9	c (t) =	56.0	c (t) =	15.4	c (t) =	15.4
Montante a investir para	MELHORAR	a (t) =		a (t) =		a (t) =		a (t) =	10,000.0	a (t) =	10,000.0	a (t) =	10,000.0

Figure 9. Decision Tree without improvement during Demonstration A Stage.

TEMPO DE DURAÇÃO DAS ETAPAS E TAXA DE DESCONTO AJUSTADA

ETAPA 1 (anos)	2.0	ETAPA 2 (anos)	1.0	ETAPA 3 (anos)	3.0	ETAPA 4 (anos)	2.0	ETAPA 5 (anos)	1.5	ETAPA 6 (anos)	1.5
Taxa Ajustada =	7.39%	Taxa Ajustada =	3.63%	Taxa Ajustada =	11.29%	Taxa Ajustada =	7.39%	Taxa Ajustada =	5.49%	Taxa Ajustada =	5.49%

INVESTIMENTO EM PESQUISA E DESENVOLVIMENTO

		INVESTIMENTO	I1	INVESTIMENTO	I2	INVESTIMENTO	I3	INVESTIMENTO	I4	INVESTIMENTO	I5	INVESTIMENTO	I6
Montante a investir para	CONTINUAR	c (t) =	0.6	c (t) =	0.2	c (t) =	3.9	c (t) =	56.0	c (t) =	15.4	c (t) =	15.4
Montante a investir para	MELHORAR	a (t) =		a (t) =		a (t) =		a (t) =	15.4	a (t) =	10,000.0	a (t) =	10,000.0

Figure 10. Decision Tree with improvement during Demonstration A Stage.

6. Conclusions

This paper analysed the decision–making process of investments in research and development (R&D) projects. A case–study of the development of a technology based on the biochemical conversion of sugarcane bagasse for the production of lignocellulosic ethanol in Brazil was presented.

From Table 10 in the previous section it is possible to see that with no decision flexibility – i.e., without active management – the value of the R&D project has the negative value of US$ –110.0 million, thus discouraging the R&D effort. However, when flexibility is possible, allowing for the options of either continuing or abandoning the project, it produces a positive value of US$ 137.83 million. Furthermore, with the added flexibility of three options (to continue, improve or abandon) the project's value is still higher, reaching US$ 166.39 million.

Therefore, the grand conclusion is that active management is a valuable asset, for it can detect promising opportunities where the orthodox approach to the valuation of a R&D project finds none.

Aknowledgements

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References

[1] Y. Liao, F. Yen, F. Hung, C. Su and W. Chen, Intermittent pressurized operation of steam explosion pretreatment system, Journal of Taiwan Institute of Chemical Engineers, vol. 67, pp. 285–291, 2016.

[2] H. Chen, J. Liu, X. Chang, D. Chen, Y. Xue, P. Liu, H. Lin and S. Han, A review on the pretreatment of lignocellulose for high–value chemicals, Fuel Processing Technology, vol. 160, pp. 196–206, 2017.

[3] D. Humbird, R. Davis , L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton and D. Dudgeon, Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute–Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover, National Renewable Energy Laboratory, Technical Report NREL/TP–5100–47764, Golden, Colorado, May 2011.

[4] T. L. Junqueira, M. F. Chagas, V. L. R. Gouveia, M. C. A. Rezende, M. D. B. Watenabe, C. D. F. Jesus, O. Cavalett, A. Y. Milanez and A. Bonomi, Techno–economic analysis and climate change impacts of sugarcane biorefineries considering different time horizons, Biotechnology for Biofuels, pp. 10–50, 2017.

[5] B. C. Klein, M. F. Chagas, T. L. Junqueira, M. C. A. F. Rezende, T. F. Cardoso, O. Cavalett and A. Bonomi, Techno–economic and environmental assessment of renewable jet fuel production in integrated Brazilian sugarcane biorefineries, Applied Energy, vol. 209, pp. 290–305, 1 January 2018.

[6] V. Hernández, J. M. Romero–Garcia, J. A. Dávila, E. Castro and Cardona C. A. , Techno–economic and environmental assessment of an olive stone based biorefinery, Resources, Conservation and Recycling, vol. 92, pp. 145–150, November 2014.

[7] Y. K. Wan, J. Sadhukhan, K. S. Ng and D. K. S. Ng, Techno–economic evaluations for feasibility of sago–based biorefinery, Part 1: Alternative energy systems, Chemical Engineering Research and Design, vol. 107, pp. 263–279, March 2016.

[8] Y. K. Wan, J. Sadhukhan and D. K. S. Ng, Techno–economic evaluations for feasibility of sago–based biorefinery, Part 2: Integrated bioethanol production and energy systems, Chemical Engineering Research and Design, vol. 107, pp. 102–116, March 2016.

[9] R. J. Stoklosa, A. P. Orjuela, L. C. Sousa, N. Uppugundla, D. L. Williams, B. E. Dale, D. B. Hodge and V. Balan, Techno–economic comparison of centralized versus decentralized biorefineries for two alkaline pretreatment processes, Bioresource Technology, vol. 226, pp. 9–17, February 2017.

[10] R. L. N. Taylor–de–Lima, A. J. G. Da Silva, L. F. L. Legey and A. Szklo, Evaluation of economic feasibility under uncertainty of a thermochemical route for ethanol production in Brazil, Energy, vol. 150, pp. 363–376, 2018.

[11] A. Arora, J. Banerjee, R. Vijayaraghavan, D. MacFarlane and A. F. Patti, Process design and techno–economic analysis of an integrated mango processing waste biorefinery, Industrial Crops and Products, vol. 116, pp. 24–34, June 2018.

[12] A. A. Longati, A. R. A. Lino, R. C. Giordano, F. F. Furlan and A. J. G. Cruz, Defining research & development process targets through retro–techno–economic analysis: The sugarcane biorefinery case, Bioresource Technology, vol. 263, pp. 1–9, September 2018.

[13] M. Mandegari, S. Farzad and J. F. Görgens, A new insight into sugarcane biorefineries with fossil fuel co–combustion: Techno–economic analysis and life cycle assessment, Energy Conversion and Management, vol. 165, pp. 76–91, 1 June 2018.

[14] A. Huchzermeier and C. H. Loch, Project Management Under Risk: Using the Real Options Approach to Evaluate, Management Science, Vols. Vol. 47(1), Design and Development, pp. 85–101, January 2001.

[15] L. P. Santiago and P. Vakili, On the Value of Flexibility in R&D Projects, Management Science, vol. 51(8), pp. 1206–1218, 2005.

[16] J. Kettunen, Y. Grushka–Cockayne and Z. Degraeve, New product development flexibility in a competitive environment, European Journal of Operational Research, vol. 244 (3), p. 892–904, 2015.

[17] J. Wang and C.–Y. Yang, Flexibility planning for managing R&D projects under risk, International Journal of Production Economics, vol. 135(2), pp. 823–831, 2012.

[18] J. Wang, C.–H. Cheng, Y.–I. Lin and C.–H. Chang, A Risk–based Real Options Framework for Flexible Technology Planning, DOI: 10.5220/0005736702790286, Proceedings of 5th the International Conference on Operations Research and Enterprise Systems (ICORES 2016), pp. 279–286, 2016

[19] N. Koussis, S. H. Martzoukos and L. Trigeorgis, Real R&D options with time–to–learn and learning–by–doing, Annals of Operations Research, vol. 151(1), pp. 29–55, 2007.

[20] F. Wu, H. Li, L. K. Chu, D. Sculli and K. Gao, An approach to the valuation and decision of ERP investment projects based on real options, Annals of Operations Research, vol. 168 (1), p. 181–203, 2009.

[21] P. C. Pendharkar, Valuing interdependent multi–stage IT investments: A real options approach, European Journal of Operational Research, vol. 201 (3), p. 847–859, 2010.

[22] Y. d'Halluin, P. Forsyth and K. Vetzal, Wireless network capacity management: A real options approach, European Journal of Operational Research, vol. 176(1), p. 584–609, 2007.

[23] L. Khansa and D. Liginlal, Valuing the flexibility of investing in security process innovations, European Journal of Operational Research, vol. 192(1), pp. 216–235, 2009.

[24] E. Pennings and L. Sereno, Evaluating pharmaceutical R&D under technical and economic uncertainty, European Journal of Operational Research, vol. 212 (2), p. 374–385, 2011.

[25] M. Valdivia, J. L. Galan, J. Laffarga and J. L. Ramos, A research and technology valuation model for decision analysis in the environmental and renewable energy sectors, Renewable and Sustainable Energy Reviews, vol. 122, pp. 109726, https://doi.org/10.1016/j.rser.2020.109726, 2020.

[26] L. A. R. Batalha, Q. Han, H. Jameel, H. Chang, J. L. Colodette and F. J. B. Gomes, Production of fermentable sugars from sugarcane bagasse by enzymatic hydrolysis after autohydrolysis and mechanical refining, Bioresource Technology, vol. 180, p. 97–105, 2015.

[27] D. Edwards, Scaling up step by step, Biofuels International, November, 2012, Available at: http://www.zeton.com/site/pdf_articles/Zeton_Scaling_Up.pdf, 2012.

[28] J. Harmsen, Industrial Process Scale–Up – A practical Innovation Guide from idea to commercial implementation, Elsevier, Amsterdam, 2013.

[29] D. R. Anderson, D. J. Sweeney, T. A. Williams, J. Camm, J. J. Cochran, M. J. Fry and J. W. Ohlmann, Decision Analysis, in Quantitative Methods for Business, Cengage Learning, South–Western, Twelfth Edition, 2013, pp. 102–156, Chap. 4.

[30] D. G. Luenberger, Investment Science, New York: Oxford University Press, Inc., 1998.

[31] L. A. M. Leite, L. P. Santiago and J. P. Teixeira, Opções reais sob Incerteza Knightiana na avaliação econômica de projetos de Pesquisa e Desenvolvimento [Real options under Knightian uncertainty for economic assessment of research and development projects], Production, vol. 25(3), pp. 641–656, jul./set. 2015.

[32] P. Crama, B. De Reyck, Z. Degraeve and W. Chong , Research and Development Project Valuation and Licensing Negotiations at Phytopharm plc., Interfaces, Vols. 37(5), Research Collection Lee Kong Chian School Of Business, pp. 472–487, 2007.

[33] J. S. Stonebraker, How Bayer Makes Decisions to Develop New Drugs, Interfaces, vol. 6 (November/December), pp. 77 – 90, 2002.

[34] M. Mitchell, The Sunliquid® Process: Bringing new proven solution for commercial cellulosic ethanol production, 25 July 2017. [Online]. Available: https://www.bio.org. [Accessed 07 April 2020].

[35] E. Johnson, Integrated enzyme production lowers the cost of cellulosic ethanol, Biofuels, Bioproducts & Biorefining, pp. 164–174, 08 February 2016.

[36] F. Marques, Obstáculos no caminho, Revista Fapesp, no. 268, June 2018.

[37] A. Sheth, Enfinity – Biomass to Ethanol Technology / Biomass to Bioethanol – Second generation technology by Praj, AIDA – All India Distillers' Association, 18 February 2016. [Online]. Available: https://www.aidaindia.org/pdf/2.pdf.

[38] A. J. G. Da Silva, Avaliação da rota termoquímica de produção de etanol e álcoois superiores [Evaluation of thermochemical route for ethanol and higher alcohols production], D.Sc. Thesis, Department of Energy Planning, Graduate School of Engineering (COPPE), The Federal University of Rio de Janeiro, Rio de Janeiro, 2013.

[39] American Association of Cost Engineers – AACE, Recommended Practice No. 18R–97, Rev. November 29, Cost EstimateClassification System – As Applied in Engineering, Procurement, and Construction for the Process Industries, AACE International, 2011.

[40] D. Voorhis, Hugoton cellulosic ethanol plant sold out of bankruptcy, 09 December 2016. [Online]. Available: https://www.kansas.com/news/business/article119902263. [Accessed 06 April 2020].

[41] Bioenergy International, POET–DSM to pause ethanol production and revert to R&D at Project LIBERTY, 21 November 2019. [Online]. Available: https://bioenergyinternational.com/biofuels–oils/poet–dsm–pause–ethanol–production–and–revert–to–rd–at–project–liberty. [Accessed 06 April 2020].

[42] Eni Press Release (February 8, 2020), Versalis–biomass–power–plant–restarted–at–crescentino–and–bioethanol–production–onstream–within–the–first–half–of–the–year, [Online]. Available: https://www.eni.com/en–IT/media/press–release/2020/02/versalis–biomass–power–plant–restarted–at–crescentino–and–bioethanol–production–onstream–within–the–first–half–of–the–year.html. [Accessed 06 April 2020].

[43] Verbio press release (November 11, 2018), Verbio–to–acquire–duponts–nevada–iowa–based–cellulosic–ethanol–plant, [Online]. Available: https://www.verbio.de/en/press/news/press–releases/verbio–to–acquire–duponts–nevada–iowa–based–cellulosic–ethanol–plant/. [Accessed 06 April 2020].

[44] H. T. Kennedy, Breaking the bottleneck – POET–DSM achieves cellulosic biofuel breakthrough, Biofuels Digest, Available at: http://www.biofuelsdigest.com/bdigest/2017/11/03/breaking–the–bottleneck–poet–dsm–achieves–cellulosic–biofuel–breakt, November 3, 2017.

[45] M. Sapp, Omega Energy and Louisiana sugar mill tap Praj to design first ethanol plant from bagasse in the US, 03 September 2019. [Online]. Available: https://www.biofuelsdigest.com/bdigest/2019/09/03/omega–energy–and–louisian–sugar–mill–tap–praj–to–design–first–ethanol–plant–from–baggase–in–the–us/. [Accessed 06 April 2020].

[46] M. Scaramuzzo and R. Agostini, GranBio: Usina hoje vende energia em vez de produzir etanol, O Estado de S. Paulo, 06 November 2017. [Online]. Available: https://www.novacana.com/n/etanol/2–geracao–celulose/granbio–usina–vende–energia–produzir–etanol–061117. [Accessed 06 April 2020].

[47] M. Rarbach, The sunliquid® Process:Proven Solutions for Advanced Biofuels in India, March 2018. [Online]. [Accessed 06 April 2020].

[48] Raízen, Raízen 2018–2019 Annual Report – We are an integrated energy company..., 24 June 2019. [Online]. Available: https://www.raizen.com.br/relatorioanual/1819/en/. [Accessed 06 April 2020].

Biographical Information

Reynaldo L. N. Taylor–de–Lima is Partner and Director at TL CONSULTORIA and Post–doctoral fellow at the Department of Energy Planning (PPE), Graduate School of Engineering (COPPE) of the Federal University of Rio de Janeiro (UFRJ). He holds a Dr.–Ing. degree in Computer Applications from the University of Stuttgart, Germany (1988). He has been Senior Analyst and Deputy Manager of the Oil Refining and Natural Gas Processing Division of the Brazilian National Petroleum Agency (ANP) and, hired as an outside specialist by José Bonifácio University Foundation (FUJB), Senior Advisor of the Biomass Conversion Division of the Petrobras Research Centre (CENPES). His present research interests include mathematical modelling for economic feasibility assessment of technologies related to oil refining, natural gas processing and biomass conversion.

Luiz Fernando Loureiro Legey is a full professor (retired) of the Energy Planning Programme of the Alberto Luiz Coimbra Institute for Graduate Studies and Research in Engineering (COPPE) of the Federal University of Rio de Janeiro (UFRJ). He holds a Ph.D. in Industrial Engineering and Operations Research from the University of California at Berkeley and has been Director of COPPE as well as Technology Director of FAPERJ (Rio de Janeiro State Foundation for the Endowment of Research). His present research interests include the mathematical modelling of energy and environment related issues.

Luiz Fernando Martins Bandeira received the B.E in Chemical Engineering from the Federal University of the State of Rio de Janeiro (UFF), Rio de Janeiro, Brazil, in 2004 and the M.S. degree in Chemical Engineering with focus on membrane separation processes and adsorption from the Federal University of Rio de Janeiro (UFRJ), Brazil, in 2007. He is a Processing Engineer of the Petrobras Research Centre (CENPES) since 2007, mainly working with second generation ethanol. He has specialization courses in oil and gas industry from the Federal University of the State of Rio de Janeiro (UFF) in 2004, from the State University of Rio de Janeiro (UERJ) in 2007, and from the Catholic University of Petropolis (UCP) in 2011. He is also a doctoral student in catalysis area at the UFRJ since 2016.

Adriano do Couto Fraga received the B.S. degree in Chemical Engineering and M.S. in Biofuels Engineering from the Federal University of Rio de Janeiro. He is Engineer at Petrobras Research and Development Centre (CENPES), where he joined in 2002. He has 15 years of experience in advanced biofuels and has been coordinating several research projects in this area. His research focus on thermochemical biomass conversion routes, as well as cellulosic ethanol.

Supplementary Appendix

Nomenclature

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X	conversion yield (litres of ethanol / dry ton of biomass)
X_T	conversion yield at the project's conclusion (litres of ethanol / dry ton of biomass)
X_{T_0}	value X_T for which $V_T(X_T) = 0$
V	project value (US$ million)
M	high extreme value achieved for $V_T(X_T)$ (US$ million)
m	low extreme value achieved for $V_T(X_T)$ (US$ million)
P_0	initial price used in the stochastic analysis (US$/litre, US$/dry ton)
$\overline{P}$	long-term price used in the stochastic analysis (US$/litre, US$/dry ton)

Greek symbols

$\bar{\tau}$	mean reverting stochastic process parameter (long-term mean, $\bar{\tau} = ln\,\overline{P}$)
η	mean reverting stochastic process parameter (speed of reversion to the mean)
σ	mean reverting stochastic process parameter (volatility)

Subscripts

t	current time
T	time of the project's conclusion

Introduction

As discussed in section 2 of the paper, the payoff $V_T(X_T)$ of the technology is described by a "generalized logistic function" defined by equation (6). However, before proceeding with the estimation of this equation, the extreme values the payoff $V_T(X_T)$, M and m, have to be computed as net present values (NPV) of the project, when yields are high and costs are low (M), and when yields are low and costs are high (m). This Supplementary Appendix presents details of how these values were calculated.

A.1 The high extreme value (M) for the payoff $V_T(X_T)$

Data provided by Humbird et al. [1A] and adapted to the Brazilian conditions is used to determine the high extreme value M for the technology payoff $V_T(X_T)$. Its computation follows the procedure for the techno-economic assessment of a thermochemical ethanol production process in Brazil outlined in Taylor-de-Lima et al. [2A]. Here it considers a commercial lignocellulosic ethanol plant with process capacity of 2,000 metric dry tons of sugarcane bagasse per day in the State of São Paulo, which are first converted into 1,007.3 tons of sugars per day and then, through fermentation, in 659,254 litres of ethanol per day, which corresponds to an approximate yield of $X_T = 390\ l/$ dry ton of sugarcane bagasse ground fibre for the high payoff

The operation of the ethanol plant under study is divided into nine large process areas, as shown in Table A1, in US dollars referred to the year 2019. The installed costs for each of these process areas and also for the Fixed Capital Investment (FCI) are referred to the United States Gulf Coast (USGC), and corresponds to US$ 511,955,281. This number, multiplied by an internalization factor of 1.7843 (Da Silva, [3A]), provides a basis for the estimation of the FCI for Brazil (FCI-BR), which amounts to US$ 913,481,808. In accordance to Table 1 of the AACE International [4A], a typical Class 3 estimate for a process industry project may have an accuracy range as broad as -20% to +30%. Thus, the FCI-BR can be as low as US$ 730,785,466 or as high as US$ 1,187,526,350. In the case of the high extreme value M, the FCI-BR will be assumed as US$ 730,785,466.

The calculation of project revenues and operating costs is based on the mass balance of Humbird et al. [1A], adapted by the authors, which discriminates the technical coefficients for products, inputs and utilities, as shown in Tables A2.a and A2.b. It considers a single price scenario for most of the variables that receive a deterministic treatment in the economic viability analysis. The constant prices of products, inputs and utilities – in 2019 US dollars– are shown in Table A3.

* Corresponding author
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Table A1. Lignocellulosic Ethanol Commercial Plant – Capital Investment.

BIOCHEMICAL ETHANOL - CAPITAL INVESTMENT (CAPEX)			
Total Investment			**Installed Costs USA (US$)**
Process Areas			
Area 100: Feedstock handling			27,777,992
Area 200: Pretreatment and conditioning			37,764,295
Area 300: Enzymatic hydrolysis na fermentation			35,812,948
Area 400: Enzyme production			21,005,672
Area 500: Destilation / Dehydration / Separation of Solids			25,597,075
Area 600: Wastewater			56,703,835
Area 700: Storage			5,739,255
Area 800: Boiler			75,758,160
Area 900: Utilities			7,920,171
ISBL (Areas 100 - 500)			**147,957,983**
OSBL (Areas 600 - 900)			**146,121,421**
Total installed cost (Area 100 excluded) (TIC)			**294,079,404**
Other direct costs			
Warehouse	(% do ISBL)	4.0%	5,918,319
Site development	(% do ISBL)	9.0%	13,316,218
Additional piping	(% do ISBL)	4.5%	6,658,109
Total direct cost (TDC)			**319,972,051**
Indirect costs	(% of TDC ex Land)		**191,983,230**
Prorated expenses		10.0%	31,997,205
Field expenses		10.0%	31,997,205
Home office and construction fees		20.0%	63,994,410
Project contingency		10.0%	31,997,205
Other costs (start-up and permits)		10.0%	31,997,205
Fixed capital investment (FCI)			**511,955,281**

Some variables in the techno-economic assessment are stochastic — namely the prices of anhydrous ethanol and sugarcane bagasse — and thus must be treated accordingly, as discussed in section A.2. Before that, however, it is necessary to estimate the initial prices P_0 to be used in the stochastic analysis. For anhydrous ethanol, the initial value P_0 is set at US$ 0.50 per litre, as shown in Table A3. This value was obtained through an estimate based on the average of anhydrous ethanol domestic prices (at producer's site) in the last quarter of 2019. A depiction of the anhydrous ethanol domestic price history is shown in Figure A1 (data provided by CEPEA / ESALQ [5A]).

Table A2.a. Lignocellulosic Ethanol – High Payoff Setting – Production.

LIGNOCELLULOSIC ETHANOL - BIOCHEMICAL ROUTE - HIGH PAYOFF SETTING - PRODUCTION						
Operational Capacity	**(dry tons / h)**	**84.0**		**Sugar production**	**(tons / d)**	**1,007.3**
Ground fibre flow rate	(dry tons / h)	70.5		Glucose	(tons / day)	647.8
Operational time	(hours / year)	8,410		Xilose	(tons / day)	359.6

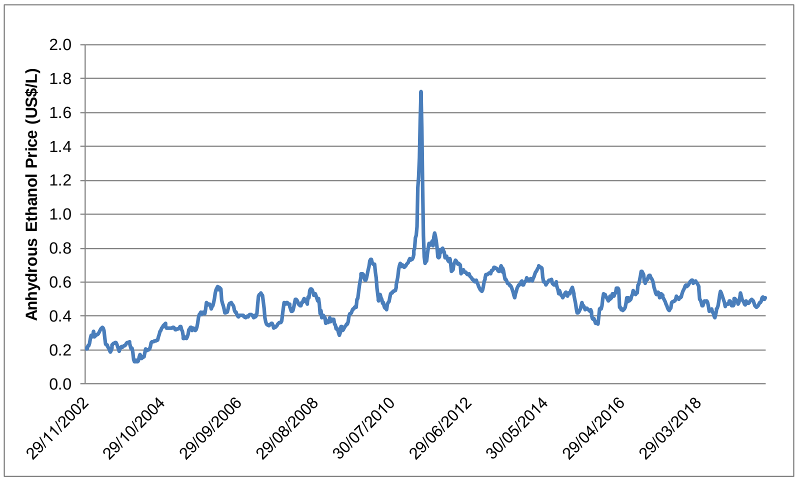
PRODUCTION PER HOUR, PER QUARTER AND PER YEAR				
Product	**Unity**	**Production (Unity / hour)**	**Production (Unity / quarter)**	**Production (Unity / year)**
Anhydrous ethanol	Litre	27,468.9	57,753,414.9	231,013,659.7
Grid electricity	kWh	12,797.0	26,905,692.5	107,622,770.0
Area 100 electricity	kWh	859.0	1,806,047.5	7,224,190.0

Table A2.b. Lignocellulosic Ethanol – High Payoff Setting – Project Consumptions.

LIGNOCELLULOSIC ETHANOL - BIOCHEMICAL ROUTE - HIGH PAYOFF SETTING - PROJECT CONSUMPTIONS				
Operational Capacity (dry tons / h)	**84.0**		**Sugar production (tons / d)**	**1,007.3**
Ground fibre flow rate (dry tons / h)	70.5		Glucose (tons / day)	647.8
Operational time (hours / year)	8,410		Xilose (tons / day)	359.6
INPUTS CONSUMPTIONS PER HOUR, PER QUARTER AND PER YEAR				
Input	**Unity**	**Production (Unity / hour)**	**Production (Unity / quarter)**	**Production (Unity / year)**
Feedstock (sugarcane bagasse)	dry ton	84.0	176,610.0	706,440.0
Sulfuric acid, 93%	Kg	1,980.6	4,164,303.0	16,657,211.9
Ammonia	Kg	1,166.0	2,451,512.9	9,806,051.8
Corn steep liquor	Kg	1,322.0	2,779,502.7	11,118,010.7
Diammonium phosphate	Kg	142.0	298,554.8	1,194,219.0
Sorbitol	Kg	44.0	92,509.9	370,039.7
Glucose	Kg	2,418.0	5,083,840.7	20,335,363.0
Sodium hydroxide (caustic soda)	Kg	3,576.3	7,519,080.4	30,076,321.4
Nutrients for enzyme production	Kg	67.0	140,867.4	563,469.5
Sulfur dioxide	Kg	16.0	33,640.0	134,559.9
FGD Lime	Kg	895.0	1,881,735.9	7,526,943.7
Boiler chemicals	Kg	0.24620	517.6	2,070.6
Cooling tower chemicals	Kg	2.38487	5,014.2	20,056.7
UTILITIES CONSUMPTIONS PER HOUR, PER QUARTER AND PER YEAR				
Utility	**Unity**	**Production (Unity / hour)**	**Production (Unity / quarter)**	**Production (Unity / year)**
Medium pressure steam	ton	0.0	0.0	0.0
Cooling water	ton	133.9	281,519.0	1,126,076.2
Boiler feed water	ton	57.4	120,651.0	482,604.1
Disposal of ash	ton	5.72500	12,036.8	48,147.3

Table A3. Lignocellulosic Ethanol – High Payoff Setting – Prices of Products, Inputs and Utilities.

PRICES OF PRODUCTS, INPUTS AND UTILITIES				
Product	**Price (2019)**	**Unity**		**Price (2007)**
Anhydrous ethanol	0.5000	(US$ / Litre)		
Grid electricity	0.0469	(US$ / kWh)		
Area 100 electricity	0.0469	(US$ / kWh)		
Input	**Price (2019)**	**Unity**	**Source**	**Price (2007)**
Feedstock (sugarcane bagasse)	8.91	(US$ / dry ton)	Taylor-deLima (2016)	
Sulfuric acid, 93%	0.1064	(US$ / ton)	NREL (2007)	0.0880
Ammonia	0.5315	(US$ / Kg)	NREL (2007)	0.4394
Corn steep liquor	0.0672	(US$ / Kg)		0.0556
Diammonium phosphate	1.1693			0.9667
Sorbitol	1.3346			1.1034
Glucose	0.6877	(US$ / Kg)	NREL (2007)	0.5686
Sodium hydroxide (caustic soda)	0.1808	(US$ / Kg)	NREL (2007)	0.1495
Nutrients for enzyme production	0.9938	(US$ / Kg)	NREL (2007)	0.8217
Sulfur dioxide	0.3675	(US$ / Kg)	NREL (2007)	0.3038
FGD Lime	0.2411	(US$ / Kg)	NREL (2007)	0.1993
Boiler chemicals	6.0428	(US$ / Kg)	NREL (2007)	4.9959
Cooling tower chemicals	3.6213	(US$ / Kg)	NREL (2007)	2.9939
Utilitiy	**Price (2015)**	**Unity**	**Source**	**Price (2007)**
Medium pressure steam		(US$ / ton)		
Cooling water	0.0591	(US$ / ton)	REPLAN (2013)	0.0532
Boiler feed water	0.2033	(US$ / ton)	REPLAN (2013)	0.1830
Disposal of ash	38.4792	(US$ / ton)	NREL (2007)	31.8127



Source: CEPEA/ESALQ (2020)[5A].

Figure A1. Anhydrous ethanol domestic market selling price.

The initial price of the sugarcane bagasse is set at US$ 8.91 per dry ton, as Table A3 shows. Its estimation was based on the opportunity cost of its use as raw material for electric energy generation (Sennejunker [6A] and Taylor-de-Lima [7A]), here considered to have been traded at US$ 46.93 per MWh, based on data provided by the 30th A-6 New Energy Auction of the Brazilian Electricity Trading Chamber (CCEE) [8A].

From the product prices in Table A3 and quantities produced in Table A2.a, it is possible to calculate the annual ethanol plant revenue (Taylor-de-Lima et al. [2A]). Similarly, annual variable costs can be calculated using Table A3 and Table A2.b. The plant annual fixed cost is divided into "Labour Costs" and "Other Fixed Costs" shown in Tables A4.a and A4.b (Humbird et al. [1A]). With these numbers, it is possible to compute the annual discounted cash flow of the project, for a 25-year period. The discount rate is set at a minimum attractiveness of 9% per year, which is the recommended value for projects that follow a sustainability bias.

Table A4.a. Lignocellulosic Ethanol – Fermentative Route – Production Fixed Costs.

LIGNOCELLULOSIC ETHANOL - ANNUAL FIXED OPERATING COSTS					
Scenario	Unique	**OPERATIONAL PHASE**			
		Year 2			
Items	**Unity**	**1rst Quarter**	**2nd Quarter**	**3rd Quarter**	**4th Quarter**
Annual Fixed Operating Costs					**28,146,967**
Labor Costs					583,108
Labor costs - Operation (4 shifts)	US$				
Labor costs - Maintenance (1,6% ISBL p.y.)	US$				
Labor costs - Laboratory (20% Labor Operation.)	US$				
Other fixed costs					27,563,859
Benefits and general (90% Labor Cost)	US$				524,798
Maintenance (3,0% FCI-BR p.y.)	US$				21,923,563
Insurance and taxes (0,7% FCI-BR p.y.)	US$				5,115,498

Table A4.b. Lignocellulosic Ethanol – Fermentative Route – Labour Costs.

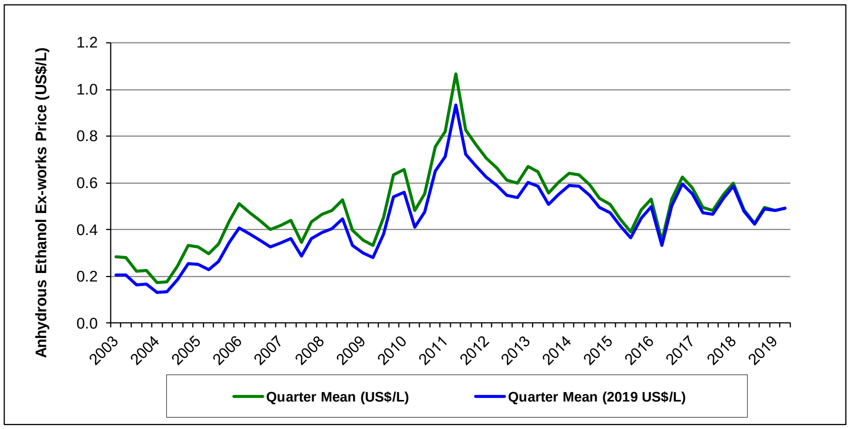
LIGNOCELLULOSIC ETHANOL - ANNUAL LABOR COSTS				
Total Labor Costs (US$ / year)			**1,090,103**	**583,108**
Position Title	**Salary (2007 US$)**	**Positions**	**Total Cost (2007 US$)**	**Total Cost (2015 US$)**
Administration			**164,153**	**87,807**
Plant manager	141,569	1	141,569	75,727
Clerks and secretaries	7,528	3	22,584	12,080
Production			**855,690**	**457,718**
Plant engineer	67,414	1	67,414	36,061
Maintenance supervisor	54,894	1	54,894	29,363
Laboratory manager	53,931	1	53,931	28,848
Shift supervisor	46,227	5	231,135	123,637
Lab technician	8,364	2	16,728	8,948
Lab technician - Enzymes	8,364	2	16,728	8,948
Maintenance technician	8,364	16	133,824	71,584
Shift operators	10,037	20	200,740	107,378
Shift operators	10,037	8	80,296	42,951
Other services			**70,260**	**37,583**
Yard employees	5,855	12	70,260	37,583

A.2 Evaluation of Economic Feasibility – Stochastic Analysis

From section A.1, initial prices P_0 are US$ 8.91 per dry ton for sugarcane bagasse and US$ 0.50 per litre for anhydrous ethanol. Under the favourable conditions assumed in the high extreme value M of the payoff $V_T(X_T)$, a 30% premium on the ethanol price will be considered or US$ 0.65 per litre. The remaining parameters $\overline{P} = \exp(\overline{\tau}), \eta$, and σ are estimated, using data from price time series shown in Figures A2 and A3 (Franco [9A] and Taylor-de-Lima et al. [2A]). Table A5 summarizes the parameter values used in the simulations, expressed in 2019 US$ deflated by the US GDP implicit price deflator [10A].

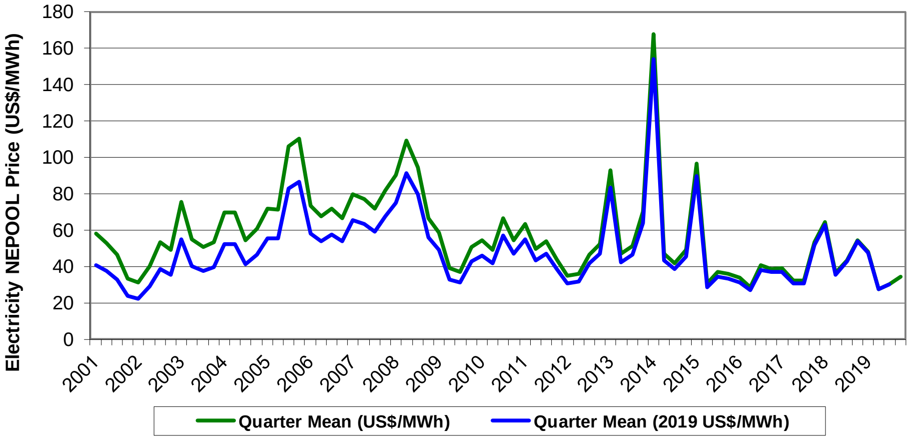
Table A5. Stochastic Modelling Parameters – Mean Reverting Process (MRP).

MRP Parameters	P_0 (2015 USD)	$\overline{P}$ (2015 USD)	η	σ
Sugarcane bagasse	8.91	7.1439	1.40946	52.760%
Anhydrous ethanol	0.500	1.0101	0.13985	33.428%



Source: CEPEA/ESALQ [5A].

Figure A2 – Anhydrous ethanol ex-works selling price (2003 – 2019).



Source: US Energy Information Administration (EIA) [11A].

Figure A3. Electricity New England Power Pool (NEPOOL) Prices (Quarter Mean).

Monte Carlo simulations were performed for 5,000 different scenarios of price trajectories for sugarcane bagasse and anhydrous ethanol. The results of the simulation are summarised in Table A6, which presents – among others – the maximum, minimum and average values of the project net present value (NPV). Results in Table A6 indicate a positive average NPV of US$ 416.0 million, with NPV positive values found in 4,950 out of 5,000 scenarios considered. In other words, the risk of finding a negative NPV is 1.0%. Thus, US$ 416.0 million is the mean value for payoff M, when conditions are most favourable. Figure A4 presents the NPV histogram obtained by simulation for the high extreme value of the payoff $V_T(X_T)$.

Table 6. Monte Carlo Simulation – Summary of 5,000 Runs (High Payoff Setting, with Premium of 30% on Ethanol Prices).

Scenario	**DISCOUNTED CASH FLOW FOR EACH SIMULATION (MM US$)**								**Risk NPV<0** **1.00%**
Items	Gross Revenue	Fixed Cost	Variable Cost	Other Expenses	Taxes	Net Income	Fixed Capital Investment	NPV	**Scenarios NPV > 0**
Minimum	657	213	274	124	11	-224	603	-441	
Maximum	3,859	213	302	124	1,025	1,953	603	1,736	**4950**
Mean	1,864	213	289	124	347	633	603	416	
1	657	213	275	124	11	-224	603	-441	0
2	936	213	290	124	48	3	603	-215	0
3	1,498	213	290	124	225	387	603	170	1
4	1,595	213	288	124	255	457	603	240	1
5	2,234	213	285	124	473	881	603	664	1
51	1,514	213	288	124	227	404	603	187	1
52	1,796	213	287	124	323	590	603	373	1
53	1,460	213	288	124	212	364	603	147	1
54	1,407	213	291	124	190	331	603	114	1
55	2,114	213	286	124	432	801	603	584	1
56	2,249	213	283	124	479	892	603	675	1
57	2,271	213	286	124	485	905	603	688	1
4,996	1,899	213	283	124	361	660	603	443	1
4,997	1,343	213	285	124	187	276	603	59	1
4,998	1,939	213	287	124	372	685	603	468	1
4,999	1,232	213	283	124	137	217	603	0	0
5,000	770	213	274	124	29	-128	603	-345	0

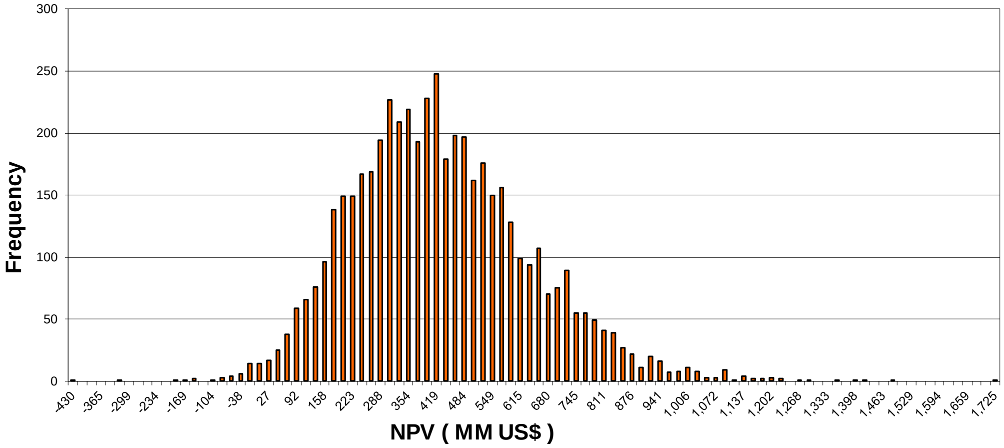


Figure A4. NPV Histogram for 5,000 runs (High Payoff Setting).

A.3 The low extreme value for the payoff $V_T(X_T)$

Similarly to the computation of the mean value for M, Monte Carlo simulations were performed in the same 5,000 different price trajectory scenarios for sugarcane bagasse and anhydrous ethanol, to determine the low value m of payoff in the most unfavourable conditions, i.e., when biomass conversion yield to ethanol has a minimum value ($X_T = 100\ l/$ dry ton of sugarcane bagasse ground fibre) and FCI-BR assumes the highest value estimated in section A.1.1, US$1,187,526,350.

The summary of this simulation is shown in Table A7. Results indicate a negative average NPV of US$ -1,293.0 million for m, with no positive NPV, which means a 100% risk of finding a negative NPV. Figure A5 presents the NPV histogram obtained in the simulation process.

Table A7. Monte Carlo Simulation – Summary of 5,000 Runs (Low Payoff Setting).

Scenario	DISCOUNTED CASH FLOW FOR EACH SIMULATION (MM US$)								Risk NPV<0 100.0%
Items	Gross Revenue	Fixed Cost	Variable Cost	Other Expenses	Taxes	Net Income	Fixed Capital Investment	NPV	Scenarios NPV > 0
Minimum	68	342	274	202	0	-1173	980	-1,496	
Maximum	1,453	342	302	202	174	31	980	-301	0
Mean	287	342	289	202	0	-964	980	-1,290	
1	68	342	275	202	0	-1168	980	-1,491	0
2	85	342	290	202	0	-1166	980	-1,490	0
3	166	342	290	202	0	-1086	980	-1,410	0
4	200	342	288	202	0	-1050	980	-1,375	0
5	450	342	285	202	0	-796	980	-1,124	0
51	191	342	288	202	0	-1059	980	-1,385	0
52	308	342	287	202	0	-941	980	-1,268	0
53	175	342	288	202	0	-1075	980	-1,400	0
54	156	342	291	202	0	-1097	980	-1,422	0
55	339	342	286	202	0	-908	980	-1,235	0
56	404	342	283	202	0	-841	980	-1,169	0
57	434	342	286	202	0	-813	980	-1,145	0
4,996	233	342	283	202	0	-1012	980	-1,336	0
4,997	136	342	285	202	0	-1110	980	-1,434	0
4,998	305	342	287	202	0	-944	980	-1,269	0
4,999	124	342	283	202	0	-1120	980	-1,444	0
5,000	68	342	274	202	0	-1167	980	-1,490	0

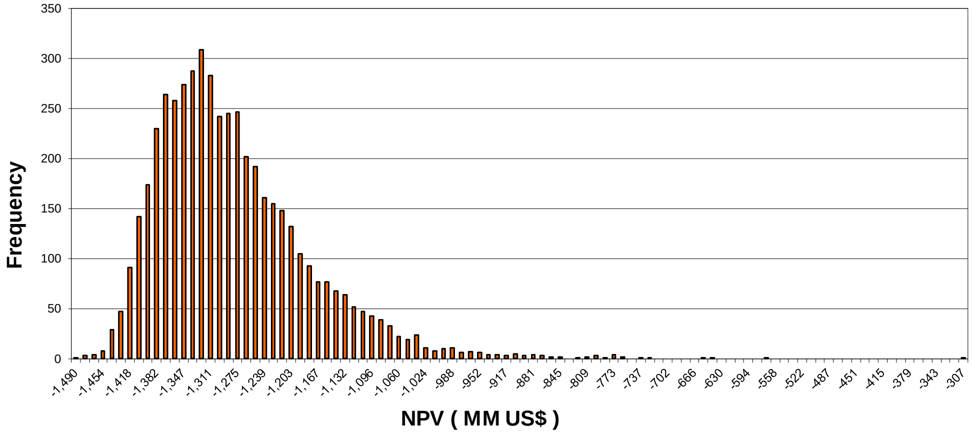


Figure A5. NPV Histogram for 5,000 runs (Low Payoff Setting).

A.4 Project Payoff Representation Through a Generalized Logistic Function

The generalized logistic function defined by equation (6) in the main paper section 2 expresses the project payoff $V_T(X_T)$. It will be adjusted so as to pass through three points: M, and m — calculated in sections A.2 and A.3, respectively — and X_{T_0} that represents the value X_T for which $V_T(X_T) = 0$, i.e., the level of performance acceptable to invest in the construction of a commercial plant.

Table A8. Generalized Logistic Function – Parameters Adjustment by Least Squares.

GENERALIZED LOGISTIC FUNCTION - PARAMETERS ADJUSTMENT BY LEAST SQUARES					
(NREL - 2000 dry tons/day, X=390 litres/dry ton + Capex Min, X=100 litres/dry ton + Capex Max)					
X	NPVobs	NPVest	NPVest–NPVobs	(NPVest-NPVobs)^2	
100	-1,290.00	-1,290.00	0.00	0.00	0.000001
240	0.00	0.00	0.00	0.00	0.000000
390	416.00	416.00	0.00	0.00	0.000001
			Summ of Squares	0.00	0.000002

The adjustment is done by the least squares method, as shown in Table A8, considering $X_{T_0} = 240\ litres/dry\ ton$; $V_T(X_T) = m$, for $X_T = 100\ litres/dry\ ton$; and $V_T(X_T) = M$, for $X_T = 390\ litres/dry\ ton$. The determined parameters are presented in Table A9 and, when substituted in equation 6, provide the generalized logistic function represented in Figure A6.

Table A9. Generalized Logistic Function – Parameters Adjusted by Least Squares.

GENERALIZED LOGISTIC FUNCTION - ESTIMATED PARAMETERS	
Parameters	Estimation
X 0 (Litres / dry tons)	240.00
m (MM US$)	-1,290.00
M (MM US$)	416.00
C	1.00000
Q	0.32248
a	0.02380
b	0.14594

	X (l / dry ton)	VT (XT) (MM US$)
6.0	400.0	416.0
5.8	395.0	416.0
5.6	**390.0**	**416.0**
5.4	385.0	416.0
5.2	380.0	416.0
5.0	375.0	416.0
4.8	370.0	416.0
4.6	365.0	416.0
4.4	360.0	416.0
4.2	355.0	416.0
4.0	**350.0**	**416.0**
3.8	345.0	416.0
3.6	340.0	416.0
3.4	335.0	416.0
3.2	330.0	416.0
3.0	325.0	416.0
2.8	**320.0**	**416.0**
2.6	315.0	416.0
2.4	310.0	416.0
2.2	305.0	416.0
2.0	**300.0**	**416.0**
1.8	295.0	415.9
1.6	290.0	415.8
1.4	285.0	415.6
1.2	280.0	415.2
1.0	275.0	414.2
0.8	**270.0**	**411.9**
0.6	265.0	406.7
0.4	260.0	395.2
0.2	255.0	369.6
0.0	**250.0**	**314.7**
-0.2	245.0	203.0
-0.4	**240.0**	**0.0**
-0.6	235.0	-303.2
-0.8	230.0	-645.5
-1.0	225.0	-928.7
-1.2	**220.0**	**-1,108.7**
-1.4	215.0	-1,204.7
-1.6	**210.0**	**-1,251.2**
-1.8	205.0	-1,272.6
-2.0	**200.0**	**-1,282.3**
-2.2	195.0	-1,286.6
-2.4	190.0	-1,288.5
-2.6	185.0	-1,289.3
-2.8	**180.0**	**-1,289.7**
-3.0	175.0	-1,289.9
-3.2	170.0	-1,289.9
-3.4	165.0	-1,290.0
-3.6	**160.0**	**-1,290.0**
-3.8	155.0	-1,290.0
-4.0	**150.0**	**-1,290.0**
-4.2	145.0	-1,290.0
-4.4	**140.0**	**-1,290.0**
-4.6	135.0	-1,290.0
-4.8	**130.0**	**-1,290.0**
-5.0	125.0	-1,290.0
-5.2	**120.0**	**-1,290.0**
-5.4	115.0	-1,290.0
-5.6	110.0	-1,290.0
-5.8	105.0	-1,290.0
-6.0	**100.0**	**-1,290.0**

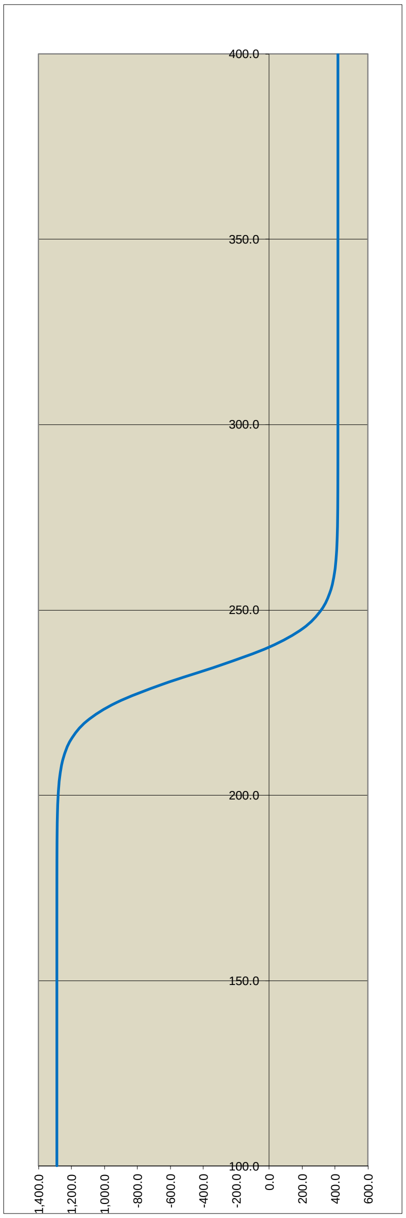


Figure A6. Generalised Logistic Function – Graphic Representation.

References

[1A] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton and D. Dudgeon, Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover, National Renewable Energy Laboratory, Technical Report NREL/TP-5100-47764, Golden, Colorado, May 2011.

[2A] R. L. N. Taylor-de-Lima , A. J. G. Da Silva, L. F. L. Legey and A. Szklo, Evaluation of economic feasibility under uncertainty of a thermochemical route for ethanol production in Brazil, Energy, vol. 150, pp. 363-376, 2018.

[3A] A. J. G. Da Slva, Avaliação da rota termoquímica de produção de etanol e álcoois superiores (Evaluation of thermochemical route for ethanol and higher alcohols production), D.Sc. Thesis, Department of Energy Planning, Graduate School of Engineering (COPPE), The Federal University of Rio de Janeiro, Rio de Janeiro, 2013.

[4A] AACE International, Recommended Practice No. 18R-97, Cost EstimateClassification System - As Applied in Engineering, Procurement, and Construction for the Process Industries, AACE International, Rev. November 29, 2011.

[5A] CEPEA/ESALQ, Série histórica de preços de etanol anidro (Price time series for anhydrous ethanol), Centre for Advanced Studies in Applied Economics, Luiz de Queiroz Superior School of Agriculture, The University of São Paulo, in www.cepea.esalq.usp.br/etanol, 2016.

[6A] K. Sennejunker, Sugar cane residues and eucalyptus wood - techno-economic analysis of availability and transport logistics for the supply of a Biomass-to-Liquid plant in southeast Brazil, M.Sc. thesis, Department of Economic and Business Engineering, Karlsruhe Institute of Technology, Karlsruhe, 2012.

[7A] R. L. N. Taylor-de-Lima, Estudo de viabilidade técnica e econômica de uma planta para produção de etanol de ligocelulose pela rota fermentativa, em D'Avila, Taylor-de-Lima, Menezes, Dalla Vechia, De Souza, Final Report of Activities, Chap. 6, Contract Petrobras Research Center Nr. 050.0092438.14.2, School of Chemistry, Federal University of Rio de Janeiro, Rio de Janeiro, 2016.

[8A] CCEE Brazilian Electricity Trading Chamber, Results of the 30th A-6 New Energy Auction, Available at: https://www.ccee.org.br/portal/faces/oquefazemos_menu_lateral/leiloes, October 18, 2019.

[9A] J. C. G. Franco, Maximum likelihood estimation of mean reverting processes, Onward Inc., in www.investmentscience.com/Content/hoetoArticles/MLE for OR mean reverting.pdf, 2013.

[10A] BEA, Gross Domestic Product: Implicit Price Deflator, National Income and Product Accounts (NIPA) Table 1.9.9, U.S. Department of Commerce: Bureau of Economic Analysis, in www.bea.gov/national, 2013.

[11A] EIA, Historical wholesale market data for electricity, New England Power Pool (NEPOOL), U.S. Energy Informationa Administration, in www.eia.gov/electricity/wholesale/, 2013.