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Exploring the evolution of biofuel supply chains
An agent-based modeling approach

Moncada Escudero, Jorge

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Exploring the Evolution of Biofuel Supply Chains

An Agent-Based Modeling Approach

EXPLORING THE EVOLUTION OF BIOFUEL SUPPLY CHAINS

AN AGENT-BASED MODELING APPROACH

Proefschrift

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus prof. dr. ir. T.H.J.J. van der Hagen,
voorzitter van het College voor Promoties,
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door

Jorge Andrés MONCADA ESCUDERO

Professional Doctorate in Engineering. Process and Equipment Design
Delft University of Technology, the Netherlands,
geboren te Puerto Salgar, Colombia.

Dit proefschrift is goedgekeurd door de

promotor: prof. dr. ir. M. P. C. Weijnen
promotor: prof. dr. ir. Z. Lukszo
promotor: prof. dr. H. M. Junginger
promotor: prof. dr. A. P. C. Faaij

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Rector Magnificus,	voorzitter
Prof. dr. ir. M. P. C. Weijnen	Technische Universiteit Delft, promotor
Prof. dr. ir. Z. Lukszo	Technische Universiteit Delft, promotor
Prof. dr. H. M. Junginger	Universiteit Utrecht, promotor
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Prof. dr. ir. W. A. H. Thissen	Technische Universiteit Delft
Prof. dr. P. Osseweijer	Technische Universiteit Delft
Prof. dr. ir. N. Shah	Imperial College London, United Kingdom
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Front & Back: The cover describes the evolution of a tree and how this process is influenced by both the provision of the right growing conditions (watering, solar radiation, and nutrients) and by the collaboration among people involved in the process. The cover was designed by Evelien Jagtman.

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to my mother and my grandmother
for teaching me what love, faith,
and courage really mean

I have tried (I am not sure how successfully) to write plain tales.
I dare not say they are simple; there is not a simple page,
a simple word, on earth—for all pages,
all words, predicate the universe,
whose most notorious attribute is complexity

Jorge Luis Borges, *Doctor Brodie's Report*

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If you want to go fast, go alone
If you want to go far, go together.

African Proverb

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Jorge A. Moncada
Leuven, September 2018

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SUMMARY

ONe of the challenges of the twenty-first century is the transition to a sustainable energy system. Road transport biofuels can play an important role in this energy transition. Indeed, biofuels have the largest global share as a mitigation measure in the road transport sector. In 2012, biofuels accounted for 3.4% of global road transport fuel demand (2.3% of total transport fuels). Biofuels are also considered as a promising strategy to decarbonize other transport sectors such as marine and aviation in the short-medium term. Nevertheless, biofuels are not cost competitive compared to fossil fuels and thus require government intervention to stimulate their production and consumption.

The policy making to stimulate the production and consumption of biofuels involves the following phases: formulation of the problem policy, policy analysis and design, policy implementation, policy evaluation, and policy maintenance or termination. Optimization/equilibrium models are increasingly being used to assist in the policy analysis and policy design supporting the expansion of biofuel supply chains. In optimization models, a central planner (e.g. government) aims to determine the optimal way to allocate resources to achieve an objective (e.g. minimization of cost) under certain constraints. These studies have provided insights as to where and when bioenergy resources and technologies can be deployed. General/partial equilibrium models are static equilibrium models of an economy. These models have the capability of explaining the consequences of changes in a particular sector in relation to the economy as a whole. General/partial equilibrium models have been used to investigate the economic consequences of further expansion of the biofuel industry around the globe.

An issue with the current models used in the policy-making to foster the biofuel sector is their inability to provide insights into the emergence of biofuel supply chains, as these models assume the existence of static equilibria. Another issue with the current models used is their lack of a realistic description of social elements such as institutional arrangements (i.e. spot market, bilateral contracts, vertical integration), social processes such as actors' decision making, and concepts such bounded rationality. Thus, these models are unable to provide insights into the role of social processes in the evolution of biofuel supply chains.

The objective of this research is to contribute to the understanding of the emergence and development of biofuel supply chains. This motivated us to formulate our research question as follows:

- *Given certain technological conditions and resources available, what institutional conditions are conducive to the emergence of a biofuel supply chain?*

The central research question was addressed within a defined geographical and temporal scope. The geographical scope consists of Germany and Brazil as these are important players on biofuels markets. The temporal scope covers the periods 2000-2014 for

the analysis of the production of biodiesel in Germany, and covers the period 2013-2030 for the analysis of the production of ethanol and biojet fuel in Brazil. The temporal scope of the Brazilian case follows from the ambition of the government of increasing the share of biofuels in the energy mix to around 18% by 2030. Three sub-questions are derived from the central research question:

1. What patterns in existing biofuel production and production capacity are generated as result of actors' behavior?

2. What patterns in existing biofuel production and production capacity emerge from different types of policy interventions?

3. What institutional conditions are conducive to the emergence of a biojet fuel supply chain from an existing road transport biofuel supply chain?

The main tenet of this dissertation is that a biofuel supply chain emerges from the interaction of social processes such as competition and collaboration among actors. Thus, to answer the research question, we developed a formal method that incorporates social processes and social structures into the analysis of biofuel supply chains. The method consists of (i) a conceptual framework and (ii) its operationalization into an agent-based model. We use agent-based modeling as a modeling paradigm because of the bottom-up perspective, adaptability, and generative nature. The objective of the conceptual framework is to assist in the construction of more comprehensive and adequate models of biofuel supply chains. The aim of the computational model is to help policy makers to formulate and assess strategies to bring biofuel supply chains into being.

We developed empirically-grounded agent-based models so as to provide insights into the processes at work in existing biofuel supply chains as these systems are site and context-specific. The models developed in this research are populated with techno-economic and geographic data, with information about policies and governance structures, and with projections for fossil fuel prices and demand of (bio) fuels. This is considered useful in the light that most agent-based models of biofuel supply chains are designed with a high level of abstraction.

At the core of the conceptual framework are three elements: the physical system, the network of actors, and institutions. The physical system refers to all physical elements in the system (infrastructure, technologies, artifacts, and resources). Actors (individuals, organizations, firms, etc.) are the entities who make decisions and participate in a process by performing a role. Finally, institutions are the customs, rules, norms, and shared strategies that shape human behavior. In this research, we assume that the behavior of the system emerges from the interactions of these elements.

The conceptual framework is underpinned by concepts derived from complex adaptive systems theory, socio-technical systems theory, and neo-institutional economics. From complex adaptive systems theory, we incorporate two elements: firstly, the tenet that system behavior in complex systems emerges from the interaction of its components. Secondly, we use core concepts of this theory such as emergence and adaptation to assist the design of the agent-based model. We follow the design principle that states that the model of a complex adaptive system, such as a biofuel supply chain, should be a complex adaptive system too. From socio-technical systems theory, we define what

elements and interactions bring about system behavior. That is, we assume that system behavior emerges from the interaction between the technical system, governed by the natural laws, and the social system, governed by institutions. Finally, from institutional economics, we use concepts from the institutional analysis framework developed by the Nobel laurate Oliver Williamson to describe how institutions influence the performance of the economy at different levels. From the same school of economic thought, we also use the concept of bounded rationality to describe actors' decision making.

The conceptual framework is used to analyze case studies and assist in the incorporation of societal processes and social structures into the design of the agent-based models. In this project we analyze three case studies: (i) production of biodiesel in Germany, (ii) production of ethanol in Brazil, and (iii) production of biojet fuel in Brazil. We started with the analysis of the German biodiesel supply chain with the aim of assessing to what extent the formal method proposed in this study provide new insights into the workings of an existing biofuel supply chain. Then, we moved into the analysis of the Brazilian ethanol supply chain as we used this biofuel supply chain as a substrate for the emergence of a biojet fuel supply chain.

The aim of the first case study was to analyze what alternative stories (scenarios) could have unfolded as a result of different policy interventions in Germany. Through this case study, we describe three methodological improvements with respect to the traditional approach in the (agent-based) modelling of biofuel supply chains. First, we present how the framework developed in this study underpinned the conceptualization of a biofuel supply chain. Second, we describe how the conceptual framework enabled the incorporation of social structures such as the spot market, social processes such as competition for feedstock, and actors' behavior such as decision making about land use into the design of a agent-based model of a biofuel supply chain. Finally, we describe how the Modeling Agent systems based on Institutional Analysis (MAIA) framework can be used to operationalize formal institutions such as blending mandates, taxes, and subsidies.

The aim of the second case study was to assess whether the Brazilian government can double the production of sugarcane-ethanol by 2030. Through this case study, we describe two methodological improvements in the modeling of biofuel supply chains. First, we introduce the spatial dimension into the agent-based modeling of biofuel supply chains as decision making about investments in processing capacity hinges on location and availability of the land to produce the feedstock. Second, we describe how to model social structures such as contracts and actors' behavior such as decision making about production and consumption of ethanol.

The aim of the third case study was to explore what institutional conditions might lead to the introduction of biojet fuel into the existing Brazilian sugarcane-ethanol supply chain. We used the model developed in the second case study as a starting point of the analysis. Through this case study, we describe how to model formal policies such as a feed-in tariff and capital investment subsidies.

Framing a biofuel supply chain as a complex adaptive system enables the incorporation of actor's processes such as adaptation, and concepts such as path dependence[1] into the analysis. Neo-institutional economics also brings new concepts such

[1] History matters; where one can go in the future hinges on what one have been in the past.

as bounded rationality and governance structures into the analysis. These concepts are rarely considered in an optimization framework. Through the case studies, we illustrate how to incorporate adaptation mechanisms and bounded rationality into the modeling of actors' behavior, and how to incorporate governance structures into the modeling of actors' interactions. When we introduced the concept of path-dependence into the analysis of the German biodiesel supply chain, we found that the timing of agricultural and biofuel policy interventions is a critical factor in shaping the evolution of the system.

Two concrete advantages of the conceptual framework are exploited when this is formalized into an agent-based model. Firstly, the computational model offers a test bed for hypotheses of system behavior. For instance, in the analysis of the German biodiesel supply chain, we found that patterns in production and production capacity observed in Germany in the period 2000-2014 are, to a certain extent, explained by the hypothesis that these patterns emerge from investors basing their decisions on optimistic perceptions of the market development. Secondly, the computational model facilitates the systematic exploration of the (consequences of the) interactions among physical components, actors, and institutions. This exploration provided insights that might underpin the future policy making to foster the emergence of new biofuel supply chains. As an illustration, in the analysis of the German biodiesel supply chain, we found that actors' adaptation mechanisms to price changes heavily influence the production of biodiesel. In the analysis of the Brazilian sugarcane-ethanol case, we found that the Brazilian government can achieve its goal of doubling the production of ethanol by 2030 by increasing the gasoline tax and abolishing the tax levied on hydrous ethanol. In this case, the model also provides insights into what data need to be collected so as to reduce the uncertainty in the gasoline tax solution space. Based on these insights, we recommend to research the mapping between gasoline tax and decision making as to ethanol production. Finally, in exploring the emergence of a biojet fuel supply chain from the existing Brazilian sugarcane-ethanol supply chain, we found that this emergence hinges on the interaction of the feed-in tariff and the gasoline tax.

This study lays out a first step in the institutional analysis of biofuel supply chains. In this research, we focused on the emergence or evolution of biofuel supply chains rather than the emergence of institutions necessary to create and develop those biofuel supply chains. Thus, from the theoretical viewpoint, we recommend further research into the co-evolution between institutions and system behavior. This avenue of research might provide insights into what conditions lead to institutional change and how this change influences the behavior of the system. The method proposed in this study along with machine learning techniques can be used for this exploration. An alternative to model the emergence of institutions is by incorporating the policymaker into the scope of the model. Machine learning techniques can be used to model the policymaker's learning processes necessary for the design and appraisal of new policy instruments.

Yet, this research is a step forward in the development of models that provide a richer description of biofuel supply chains. The agent-based models developed in this research illustrate how to incorporate the effect of actors' preferences in their decision making, how to include governance structures, and how to map biofuel policies onto actor behavior. Notwithstanding their importance, these elements are neglected by mainstream approaches. Finally, given that biofuel supply chains are complex and context-dependent,

we argue that we should strive for both developing models that incorporate the necessary causal mechanisms for a reliable description of the problem at hand and, if necessary, integrating models that describe biomass/biofuel markets in different geographies. The multimodel ecology approach may be useful to facilitate model integration. The richness of socio-technical systems cannot be compressed into one unique modeling paradigm.

SAMENVATTING

Eén van de uitdagingen van de eenentwintigste eeuw is de transitie naar een duurzaam energiesysteem. Biobrandstoffen voor wegtransport kunnen hierin een belangrijke rol spelen. Biobrandstoffen hebben wereldwijd het grootste aandeel in maatregelen ter verduurzaming van de wegtransportsector. In 2012 namen biobrandstoffen 3.4% van de wereldwijde vraag naar wegtransportbrandstof voor hun rekening (2.3% van de totale vraag naar transportbrandstoffen). Biobrandstoffen worden ook beschouwd als een veelbelovende strategie om andere transportsectoren zoals de zeescheepvaart en luchtvaart te verduurzamen. Desalniettemin zijn biobrandstoffen niet kostencompetitief vergeleken met fossiele brandstoffen, en vergen daarom overheidsingrijpen om de productie en consumptie ervan te stimuleren.

De beleidsvorming ter stimulering van de productie en consumptie van biobrandstoffen omvat de volgende fases: formulering van het probleembeleid, beleidsanalyse en –ontwerp, beleidsuitvoering, beleidsevaluatie, en beleidsinstandhouding of –stopzetting. Optimalisatie/evenwichtsmodellen worden steeds vaker gebruikt om bij te dragen aan de analyse en het ontwerp van beleid om de uitbreiding van biobrandstofketens te ondersteunen. In optimalisatiemodellen streeft een centrale planner (bijv. de overheid) naar het vaststellen van de optimale wijze van toewijzing van grondstoffen om een doelstelling (bijv. kostenminimalisatie) te bereiken onder bepaalde randvoorwaarden. Deze studies hebben inzichten opgeleverd over waar en wanneer bio-energiegrondstoffen en –technologieën kunnen worden ingezet. Algemene/partiële evenwichtsmodellen zijn statische evenwichtsmodellen van een economie. Deze modellen worden gebruikt om de gevolgen van veranderingen in een specifieke sector in relatie tot de algehele economie te verklaren. Algemene/partiële evenwichtsmodellen zijn ingezet om de economische gevolgen van uitbreiding van de biobrandstofindustrie in de wereld te onderzoeken.

Een aandachtspunt bij de huidige modellen die gebruikt worden in beleidsvorming ter stimulering van de biobrandstofsector, is hun onvermogen om inzicht te geven in de emergentie van biobrandstofketens, aangezien deze modellen uitgaan van statische evenwichten. Een ander aandachtspunt bij de huidige modellen is hun gebrek aan een realistische beschrijving van sociale elementen zoals institutionele structuren (bijv. de spotmarkt, bilaterale contracten, verticale integratie), sociale processen zoals de besluitvorming van actoren, en concepten zoals beperkte rationaliteit. Daarom kunnen deze modellen geen licht werpen op de rol van sociale processen in de evolutie van toeleveringsketens voor biobrandstoffen.

Het doel van dit onderzoek is meer inzicht te creëren in de ontwikkeling van biobrandstofketens, uitgaande van de volgende onderzoeksvraag:

- *Gegeven bepaalde technologische condities en beschikbare grondstoffen, welke institutionele condities zijn bevorderlijk voor de emergentie van een biobrandstoftoe-*

leveringsketen?

De centrale onderzoeksvraag werd behandeld binnen een beperkte geografische en temporele scope. De geografische selectie betreft Duitsland en Brazilië, omdat zij belangrijke spelers in biobrandstofmarkten zijn. De temporele afbakening beslaat de periode 2000-2014 voor de analyse van de productie van biodiesel in Duitsland, en de periode 2013-2030 voor de analyse van de productie van bioethanol en biovliegtuigbrandstof in Brazilië. Laatstgenoemde keuze hangt samen met de ambitie van de Braziliaanse regering om het aandeel van biobrandstoffen in de energiemix te vergroten naar circa 18% in 2030. Drie onderliggende vragen zijn afgeleid uit de centrale onderzoeksvraag:

1. Welke patronen in bestaande biobrandstofproductie en productiecapaciteit worden gecreëerd als gevolg van het gedrag van actoren?

2. Welke patronen in bestaande biobrandstofproductie en productiecapaciteit komen voort uit verschillende typen beleidsinterventies?

3. Welke institutionele condities zijn bevorderlijk voor de emergentie van een toeleveringsketen voor biovliegtuigbrandstof uit een bestaande toeleveringsketen voor wegtransportbiobrandstof?

In de kern gaat dit proefschrift uit van de stelling dat een biobrandstofketen ontstaat uit de interactie tussen sociale processen zoals concurrentie en samenwerking tussen actoren. Daarom hebben we, om de onderzoeksvraag te beantwoorden, een formele methode ontwikkeld die sociale processen en sociale structuren meeneemt in de analyse van biobrandstofketens. De methode bestaat uit (i) een conceptueel raamwerk en (ii) de operationalisering daarvan in de vorm van een agent-gebaseerd model. We gebruiken agent-gebaseerd modelleren als modelleerparadigma vanwege het bottom-up-perspectief, de adaptiviteit, en de generatieve aard. Het doel van het conceptuele raamwerk is om te helpen bij de constructie van rijkere modellen van biobrandstofketens. Doel van het rekenmodel is om beleidsmakers te helpen bij het formuleren en evalueren van strategieën om toeleveringsketens voor biobrandstoffen tot stand te brengen.

We hebben empirisch onderbouwde agent-gebaseerde modellen ontwikkeld, zodat we inzichten kunnen leveren in de werkzame processen in bestaande biobrandstofketens, daar deze systemen plaats- en contextgebonden zijn. De in dit onderzoek ontwikkelde modellen worden gevoed met techno-economische en geografische data, met informatie over beleidsstrategieën en governance-structuren, en met projecties van fossiele brandstofprijzen en (bio)brandstofvraag. Dit wordt gezien als een nuttige en gewenste uitbreiding van het bestaande palet van agent-gebaseerde modellen van biobrandstofketens, die meestal gekenmerkt worden door een hoger abstractieniveau.

De kern van het conceptuele raamwerk bevat drie elementen: het fysieke systeem, het actorennetwerk en instituties. Het fysieke systeem verwijst naar alle fysieke elementen in het systeem (infrastructuur, technologieën, artefacten en grondstoffen). Actoren (individuen, organisaties, bedrijven etc.) zijn de entiteiten die besluiten nemen en een rol vervullen in sociale processen. De instituties tenslotte zijn de gebruiken, regels, normen en gedeelde strategieën die het gedrag van de actoren vormgeven. In dit onderzoek

nemen we aan dat het gedrag van het systeem ontstaat uit de interacties tussen deze elementen.

Het conceptuele raamwerk wordt ondersteund door concepten die zijn afgeleid uit de theorie van complexe adaptieve systemen, de theorie van socio-technische systemen en de neo-institutionele economie. Uit de theorie van complexe adaptieve systemen nemen we twee elementen op: Ten eerste, het principe dat systeemgedrag in complexe systemen ontstaat uit de interactie tussen hun componenten. Ten tweede gebruiken we kernconcepten van deze theorie zoals emergentie en adaptatie om het ontwerp van het agent-gebaseerde model te ondersteunen. We volgen het ontwerpprincipe dat stelt dat het model van een complex adaptief systeem, zoals een biobrandstofketen, ook een complex adaptief systeem zou moeten zijn. Vanuit de theorie van socio-technische systemen bepalen we welke elementen en interacties tot systeemgedrag leiden. Dat wil zeggen, we nemen aan dat systeemgedrag ontstaat uit de interactie tussen het technische systeem, onderworpen aan de natuurwetten, en het sociale systeem, onderworpen aan instituties. Ten slotte gebruiken we uit de neo-institutionele economie concepten van het institutionele analyseraamwerk ontwikkeld door de Nobel-laureaat Oliver Williamson om te beschrijven hoe instituties de prestatie van de economie beïnvloeden op verschillende niveaus. Uit hetzelfde economische gedachtegoed gebruiken we ook het concept van beperkte rationaliteit om de besluitvorming van actoren te beschrijven.

Het conceptuele raamwerk wordt gebruikt om case studies te analyseren en te helpen bij de representatie van maatschappelijke processen en sociale structuren in het ontwerp van de agent-gebaseerde modellen. In dit project analyseren we drie cases: (i) productie van biodiesel in Duitsland, (ii) productie van ethanol in Brazilië, en (iii) productie van biovliegtuigbrandstof in Brazilië. We begonnen met de analyse van de Duitse biodieselketen met het doel om te beoordelen in hoeverre de formele methode zoals voorgesteld in deze studie, nieuwe inzichten kan opleveren in het functioneren van een bestaande biobrandstofketen. Daarna stapten we over op de analyse van de Braziliaanse bio-ethanolketen, omdat we deze biobrandstofketen als uitgangssituatie hebben gebruikt voor de emergentie van een toeleveringsketen van biovliegtuigbrandstof.

Het doel van de eerste casus was om te analyseren welke alternatieve scenario's zich hadden kunnen ontvouwen als Duitsland andere beleidsinterventies had toegepast. Deze casus bracht ons drie methodologische verbeteringen ten aanzien van de traditionele aanpak van het (agent-gebaseerd) modelleren van biobrandstofketens. Ten eerste laten we zien hoe het raamwerk dat in deze studie is ontwikkeld de conceptualisatie van een biobrandstofketen heeft ondersteund. Ten tweede beschrijven we hoe het conceptuele raamwerk het mogelijk maakte om sociale structuren zoals de spotmarkt, sociale processen zoals concurrentie om grondstoffen, en gedrag van actoren zoals besluitvorming over landgebruik, mee te nemen in het ontwerp van een agent-gebaseerd model van een biobrandstofketen. Tot slot beschrijven we hoe het 'Modeling Agent systems based on Institutional Analysis (MAIA)'- raamwerk gebruikt kan worden om formele instituties zoals mandaten, belastingen en subsidies, in een agent-gebaseerd model te operationaliseren.

Het doel van de tweede casus was om te beoordelen of de Braziliaanse overheid de productie van suikerriet-ethanol kan verdubbelen voor 2030. Deze casus bracht ons tot twee nieuwe methodologische verbeteringen voor het modelleren van biobrandstofke-

tens. Ten eerste introduceren we de ruimtelijke dimensie in het agent-gebaseerd modelleren van biobrandstofketens, omdat besluitvorming over investeringen in verwerkingscapaciteit afhangt van de locatie en de beschikbaarheid van land om de grondstoffen te produceren. Ten tweede laten we zien hoe sociale structuren zoals contracten en het gedrag van actoren in de besluitvorming over productie en consumptie van ethanol kunnen worden gemodelleerd.

Het doel van de derde casus was om te verkennen welke institutionele condities zouden kunnen leiden tot de introductie van biovliegtuigbrandstofproductie in de bestaande leveringsketen van Braziliaanse suikerriet-ethanol. We hebben het model voor de Braziliaanse bio-ethanolcasus gebruikt als startpunt van de analyse. In deze derde casus laten we zien hoe formele beleidsinstrumenten zoals een invoedingstarief en kapitaalinvesteringssubsidies kunnen worden gemodelleerd.

Het benaderen van een biobrandstofketen als een complex adaptief systeem maakt het mogelijk om adaptatieprocessen (door actoren) en concepten als padafhankelijkheid[1] in de analyse te incorporeren. Neo-institutionele economie brengt ook nieuwe concepten in de analyse, zoals beperkte rationaliteit en governance-structuren. Deze concepten worden zelden opgenomen in een optimalisatieraamwerk. Door middel van de case studies illustreren we hoe adaptatiemechanismes en beperkte rationaliteit kunnen worden opgenomen in het modelleren van gedrag van actoren, en hoe governancestructuren kunnen worden opgenomen in het modelleren van interacties tussen actoren. Bij toepassing van het concept van padafhankelijkheid in de analyse van de Duitse biodieselketen, stelden we vast dat de timing van beleidsinterventies, zowel op het gebied van landbouwbeleid als biobrandstofbeleid een kritieke factor is die in hoge mate bepalend is voor de evolutie van het systeem.

Twee concrete voordelen van het conceptuele raamwerk worden benut bij de formalisatie ervan in een agent-gebaseerd model. Ten eerste biedt het rekenmodel een testbed voor hypotheses over systeemgedrag. Zo stelden we in de analyse van de Duitse biodieselketen vast dat patronen in productie en productiecapaciteit, waargenomen in Duitsland in de periode 2000-2014, tot op zekere hoogte worden verklaard door de hypothese dat deze patronen hun oorsprong vinden bij investeerders die hun beslissingen baseren op optimistische percepties van de ontwikkeling van de markt. Ten tweede faciliteert het rekenmodel een systematische verkenning van de (consequenties van de) interacties tussen de fysieke componenten, actoren en instituties. Deze verkenning leverde inzichten op die de toekomstige beleidsvorming ter bevordering van de emergentie van nieuwe biobrandstoftoeleveringsketens kunnen ondersteunen. Ter illustratie, in de analyse van de Duitse biodieselketen stelden we vast dat de adaptatiemechanismen van actoren voor prijsveranderingen van grote invloed zijn op de productie van biodiesel. In de analyse van de Braziliaanse suikerriet-ethanolcasus vonden we dat de Braziliaanse overheid haar doel om de productie van ethanol voor 2030 te verdubbelen, slechts kan behalen door de benzinebelasting te verhogen en de belasting op natte (hydrous) ethanol op te heffen. In deze casus geeft het model ook in welke data verzameld moeten worden om de onzekerheid in de oplossingsruimte voor de benzinebelasting te verminderen. Gebaseerd op deze inzichten bevelen we aan om de relatie tussen benzinebelasting en besluitvorming

[1] De geschiedenis doet ertoe; waar men naar toe kan gaan in de toekomst hangt af van wat men was in het verleden.

over ethanolproductie te onderzoeken. Ten slotte laat onze verkenning van de institutionele condities waaronder een leveringsketen voor biovliegtuigbrandstof zou kunnen ontstaan uit de bestaande Braziliaanse toeleveringsketen van bio-ethanol, zien dat deze emergentie afhangt van de interactie tussen het invoedingstarief en de benzinebelasting.

Met deze studie is een eerste stap gezet in de institutionele analyse van biobrandstofketens. In dit onderzoek richtten we ons op de emergentie of evolutie van biobrandstofketens in plaats van op de emergentie van instituties die nodig zijn om zulke biobrandstofketens tot ontwikkeling te doen komen. Vanuit theoretisch perspectief bevelen we daarom verder onderzoek aan naar de co-evolutie van instituties en systeemgedrag. Deze onderzoeksrichting zou inzichten kunnen genereren over welke condities tot institutionele verandering leiden en hoe deze verandering het systeemgedrag beïnvloedt. Voor een dergelijke verkenning kan de in dit onderzoek gebruikte methode worden gecombineerd met 'machine learning'-technieken. Een alternatief voor het modelleren van de emergentie van instituties is het opnemen van de beleidsmaker als endogene actor in het model. Machine-learning-technieken kunnen worden gebruikt om de leerprocessen van de beleidsmaker, nodig voor het ontwerp en de taxatie van nieuwe beleidsinstrumenten, te modelleren.

Desondanks betekent dit onderzoek een stap vooruit in de ontwikkeling van modellen die een rijkere beschrijving van biobrandstoftoeleveringsketens geven. De agentgebaseerde modellen die zijn ontwikkeld in dit onderzoek, illustreren hoe voorkeuren van actoren kunnen worden meegenomen in hun besluitvorming, hoe governance structuren kunnen worden opgenomen, en hoe het effect van biobrandstofbeleid op het gedrag van actoren kan worden toegevoegd. Ondanks het belang van deze elementen worden ze in de gangbare modellen genegeerd. Gegeven het feit dat biobrandstofketens complex en contextafhankelijk zijn, besluiten we met een pleidooi voor het ontwikkelen van modellen die de noodzakelijke causale mechanismen incorporeren voor een betrouwbare beschrijving van het voorliggende probleem, en voor het integreren van modellen van biomassa/biobrandstofmarkten in verschillende regio's. De 'multimodel-ecologie'-aanpak kan daarbij nuttig zijn. De rijkheid van socio-technische systemen kan niet worden samengeperst in één uniek modelleerparadigma.

1

Introduction

The objective of scientific research
is not just to arrive at predictions:
it is to understand how the world functions;
to construct and develop an image of the world,
a conceptual structure to enable us to think about it.
Before being technical, science is visionary.

Carlo Rovelli, *Reality is not what it seems: the journey to quantum gravity*

There is no learning without having to pose a question.
And a question requires doubt.

Richard P. Feynman

1

1.1. MOTIVATION

ENERGY is the oxygen of the economy. Societies have come to rely on different energy sources to meet their basic requirements. These energy sources include the sun, wind, water, biomass, nuclear energy, and fossil fuels. The introduction of fossil fuels as a main source of energy boosted everything: agriculture, transportation, urbanization, quality of life, politics, and the environment [1]. Nevertheless, this development comes with a price: the current fossil energy systems are simply unsustainable from the societal, economic, and environmental viewpoint [2].

One of the challenges of the twenty-first century is to bring about a new energy transition towards a more sustainable energy system *"characterized by universal access to energy services, and security and reliability of supply from efficient, low carbon sources"* [3]. Road transport biofuels can contribute to this energy transition. Indeed, biofuels have the largest global share as a mitigation measure in the road transport sector. In 2012, biofuels accounted for 3.4% of global road transport fuel demand (2.3% of total transport fuels) [4]. This amounts to a global consumption of biofuels less than $3\,\mathrm{EJ\,yr^{-1}}$ [5]. According to the International Energy Agency (IEA), this consumption could increase by 10 times by 2050 [6]. After 2050, so as to stay on a 2 °C pathway, the levels of biofuel consumption must keep increasing as fossil fuels are phased out [7].

In Brazil, sugarcane-ethanol and biodiesel are important elements of the strategy to decarbonize the road transport sector [8, 9]. In 2014, the consumption of biofuels in Brazil amounted to approximately 23% of all transportation fuels [10]. In December 2017, the Brazilian government committed to increase the share of biofuels in the energy matrix to 18% by 2030 [11]. In June 2018, Brazil's National Council for Energy Policy (CNPE) approved a 10% carbon intensive reduction target for its transport fuel matrix by 2028 [12].

In Germany, biofuels have been a cornerstone in the strategy to decarbonize the road transport sector. In 2012, Germany was the second largest producer of biodiesel (after the United States) with a volume of 3.1 Billion liters [5]. In 2016, biofuels contributed to 6% greenhouse gas emissions (GHG) savings in the transport sector [13].

Biofuels are also considered as a promising strategy to decarbonize other transport sectors such as marine and aviation in the short-medium term [14]. The aviation industry accounts for more than 2% of global CO_2 emissions [15]. GHG emissions are projected to increase 3.6- to 6.2-fold by 2050 relative to 2010 because of the rapid growth of the aviation industry. Nevertheless, unlike for the road transport sector, short-term options to decarbonize the air transport are limited. Aviation will rely on liquid fuels with high energy density for decades to come [16]. Thus, biojet fuel is expected to make an essential contribution to the decarbonization of the aviation sector [17].

Despite the potential contribution of biofuels in the energy transition, biofuel production is not cost-competitive and thus requires governmental intervention. Policy instruments such as tax exemptions, subsidies, blending mandates, and import tariffs are used by governments around the world to stimulate production and increase consumption of biofuels [18].

The policy-making to stimulate the production and consumption of biofuels involves the following phases: formulation of the problem policy, policy analysis and design, policy implementation, policy evaluation, and policy maintenance or termination. Opti-

mization/equilibrium models are increasingly being used to assist in the policy analysis and policy design supporting the expansion of biofuel supply chains. These models have provided insights into the location and scale of biofuel production plants and environmental performance of biofuel supply chains [19–21]. Nevertheless, these models are unable to provide insights into the role of social processes in the evolution of biofuel supply chains.

Understanding the emergence of biofuel supply chains plays an important role in the decarbonisation of the transport sector (road, aviation, and maritime), for the gained insights may lead to the design of more effective policy instruments to stimulate production and consumption of biofuels.

Biofuels can play an important role in the years to come in the decarbonisation of the transport and energy sector. To foster the development of biofuel supply chains, it is paramount both to enhance policy support and to increase the effectiveness of the policy analysis and design. The effectiveness of the designed policy instruments can be increased by providing insights into what processes and mechanisms influence in the emergence of biofuel supply chains. Once we understand how biofuel supply chains come into being, we can foster and improve the emergence of these systems by tweaking the technological, economic, and institutional conditions.

The remainder of the chapter is organized as follows: Section 1.2 discusses the state of the art in the modeling of biofuel supply chains. Section 1.3 presents the objective of this dissertation and the research questions to be addressed. The research approach is presented in Section 1.4. Section 1.5 describes the scope of this research project. Finally, Section 1.6 presents the outline of the dissertation.

1.2. STATE OF THE ART IN THE MODELING OF BIOFUEL SUPPLY CHAINS

OPTIMIZATION/equilibrium models are increasingly being used to underpin the policy-making to foster the emergence and development of biofuel supply chains. The following subsection outlines the status of knowledge on the modeling of biofuel supply chains.

1.2.1. MODELLING OF BIOFUEL SUPPLY CHAINS

In optimization models, a central planner (e.g. government) aims to determine the optimal way to allocate resources to achieve an objective (e.g. minimization of cost) under certain constraints. These studies have provided insights as to where and when bioenergy resources and technologies can be deployed [19–21]. General/partial equilibrium models are static equilibrium models of an economy [22]. These models have the capability of explaining the consequences of changes in a particular sector in relation to the economy as a whole [23]. General/partial equilibrium models have been used to investigate the economic consequences of further expansion of the biofuel industry around the globe [24–27].

An issue with the current models used in the policy-making to foster the biofuel sector is their inability to provide insights into the emergence of biofuel supply chains, as these models assume the existence of static equilibria. Another issue with the current

models used is their lack of a realistic description of social elements such as institutional arrangements (i.e. spot market, bilateral contracts, vertical integration) and social processes such as actors' decision making.

As pointed out in the literature focused on organizational theory, the economic performance of biofuel supply chains also depends on institutional arrangements. The organization of the biofuel supply chain is relevant for at least three reasons. First, specialized investments in technology to process biomass creates a bilateral dependence between otherwise independent actors [28]. Second, the organization of the biofuel supply chain affects the long-term economic performance of biofuel plants. Finally, the organization of the biofuel supply can produce harmful environmental consequences (e.g. an additional ecological load on the land) [29].

Moreover, the behavior of the biofuel supply chain is by large driven by decision making about investment in, production of, and consumption of biofuels. Nevertheless, the process of decision making is seldom considered in the modeling of biofuel supply chains. If this process is explicitly incorporated into the modeling, it is under the assumption that actors are rational and have an unlimited capacity for processing information [30]. Behavioral economists, however, have demonstrated that the rationality in human beings' decision making is bounded [31].

Recently, other modelling paradigms such as system dynamics (SD) and agent-based modelling (ABM) have been used in the modelling of biofuel supply chains. Compared to optimization models, however, the use of SD and ABM to inform policymaking is still limited. System dynamics is a modelling technique used to analyse complex systems. This approach is based on the idea that the behaviour of the system is largely influenced by the system structure, which can create feedback loops and time delays. The formalization of these models is characterized by the use of variables such as stocks and flows [32]. System dynamics models have been used to gain insight into the long-term behaviour of the biofuel sector in Latvia [33] and to explore the effect of policies on the development of the ethanol industry in Brazil [34], the biodiesel industry in Colombia [35], and the fuel market in the US [36]. Nevertheless, none of these studies have explored the emergence of biofuel supply chains as SD assumes a fixed structure of the system.

Agent-based modelling is a computational technique that describes the phenomenon in terms of unique and autonomous agents that interact with each other and their environment [37]. Agent-based models have been used to provide insights into the effect of actors' behaviour and interaction on the behaviour of (or parts of) the biofuel supply chain [38, 39]. Other studies combine agent-based modelling with other techniques to provide insights into the design of bioenergy systems [40]. Several authors have used agent-based modelling to explore the effect of either formal constraints or informal constraints, such as norms of behaviour and conventions, or both on the behaviour of a biofuel supply chain [41–43]. Nevertheless, few studies have used a coherent framework that guides the conceptualization of the effect of both institutions and actors' behaviour on system's behaviour. Despite the potential of ABM of exploring emergent behaviour because of its bottom-up approach, ABM have not been used to explore the emergence of biofuel supply chains.

1.3. PROBLEM DESCRIPTION, STUDY OBJECTIVES, AND RESEARCH QUESTIONS

SCIENTIFIC literature largely focuses on the optimization problem of a biofuel supply chain. This approach has provided insights into the optimal pathway towards a desired future state (e.g. increase the share of biofuels in the energy mix). Nevertheless, it is unable to shed light on the mechanisms that lead to the emergence of a biofuel supply chain, as this approach use models that assume the existence of static equilibria [44] or assume that the dynamics of the system is governed by the predetermined system structure [45]. Moreover, these models provide, if any, an unrealistic description of social elements and social structure. Thus, the effect of institutions (i.e. formal policies, institutional arrangements, and actors' strategies) on the emergence of biofuel supply chains is still not well understood.

The objective of this research is to contribute to an understanding of the emergence and development of biofuel supply chains. This objective leads to formulate the central research question as follows:

- *Given certain technological conditions and resources available, what institutional conditions are conducive to the emergence of a biofuel supply chain?*

The central research question will be addressed within a defined geographical and temporal scope. The geographical scope of this dissertation consists of Germany and Brazil as these are important players on biofuels markets. The temporal scope covers the periods 2000-2014 for the analysis of the production of biodiesel in Germany, and covers the period 2013-2030 for the analysis of the production of ethanol and biojet fuel in Brazil. The temporal scope of the Brazilian case follows from the ambition of the government of increasing the share of biofuels in the energy mix to around 18% by 2030. Three sub-questions are derived from the central research question:

1. What patterns in existing biofuel production and production capacity are generated as result of actors' behavior?

2. What patterns in existing biofuel production and production capacity emerge from different types of policy interventions?

3. What institutional conditions are conducive to the emergence of a biojet fuel supply chain from an existing road transport biofuel supply chain?

Table 1.1 presents an overview of the dissertation chapters and their relation to the research questions.

1.4. RESEARCH APPROACH

THE overall research process is illustrated in Figure 1.1. To answer the aforementioned questions, we will develop a formal method for analysis of biofuel supply chains that incorporates the interaction of social processes, such as collaboration and competition among actors, with processes governed by the laws of nature, such as the production of

Table 1.1: Overview of the dissertation chapters and their relation to the research questions

	Chapter	Research question		
		I	II	III
3	Modeling the German biodiesel supply chain	X		
4	Institutional analysis of the German biodiesel supply chain		X	
5	Institutional analysis of the Brazilian ethanol supply chain		X	
6	Exploring the emergence of a biojet fuel supply chain			X

biofuels. The method consists of (i) a conceptual framework and (ii) its operationalization into an agent-based model. We will select a number of social theories and frameworks to provide an overall description of biofuel supply chains. These theories and frameworks will be used to develop a conceptual framework. The objective of the conceptual framework is to assist in the construction of more comprehensive and adequate models of biofuel supply chains. The aim of the computational model is to provide insights into the workings of biofuel supply chains.

Cases studies in this dissertation cover the German biodiesel supply chain and the Brazilian ethanol supply chain. The first case study deals with the production of biodiesel in Germany. The aim of this study was threefold: first, identify what policy instruments were used to stimulate the production and consumption of biodiesel; second, formalize those instruments into an agent-based model; finally, validate the proposed method by reproducing relevant historical trends. The second case study explores the effect of formal policies (i.e. blend mandates, taxes levied on gasoline, hydrous and anhydrous ethanol) on the evolution of the Brazilian ethanol market. The aim of this case study, besides providing insights into the workings of the ethanol supply chain, is to serve as a substrate for the emergence of a biojet fuel supply chain. The aim of the third case study is to explore the institutional conditions that may support the emergence of a biojet fuel supply chain into the existing Brazilian ethanol supply chain. Finally, we will conclude by reflecting on our findings.

In the next subsections, we will briefly discuss the approach adopted for this study. For a more detailed discussion, the reader is referred to Chapter 2.

1.4.1. BIOFUEL SUPPLY CHAINS AS COMPLEX ADAPTIVE SYSTEMS

According to John H. Holland, a Complex Adaptive System (CAS) can be defined as: *"[...] a dynamic network of many agents (which may represent cells, species, individuals, firms, nations) acting in parallel, constantly acting and reacting to what the other agents are doing. The control of a complex adaptive system tends to be highly dispersed and decentralised. If there is to be any coherent behaviour in the system, it has to arise from competition and cooperation among the agents themselves. The overall behaviour of the system is the result of a huge number of decisions made every moment by many individual agents"* [46]. That is, a CAS features emergent behavior.

Biofuel supply chains can be classified as complex adaptive systems. These systems are complex as firstly, they consist of a network of interacting agents. Biofuel supply

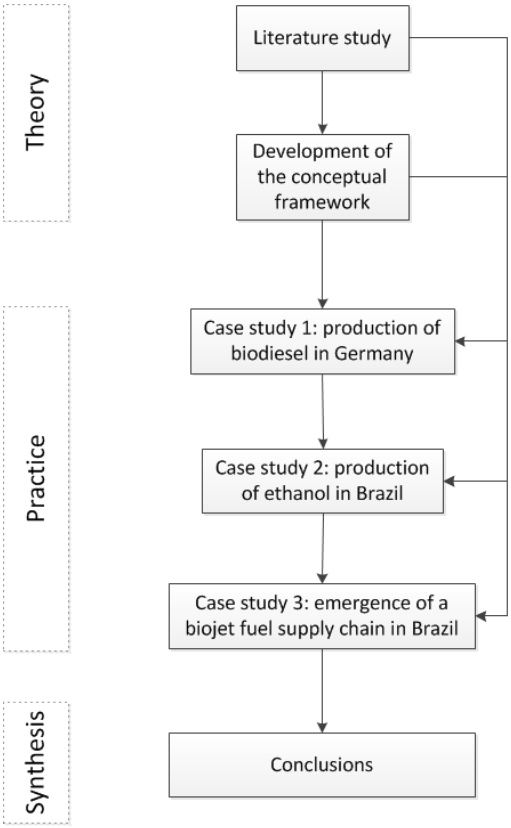

Figure 1.1: The research process.

chains consist of agents such as farmers, biofuel producers, biofuel distributors and end users. These agents form networks whereby they exchange information, mass, energy, and money. Secondly, biofuel supply chains exhibit a dynamic behaviour that emerges from the individual activities of the agents. Prices of biomass and biofuels are largely determined by the decision making of different agents in the supply chain as to investment in, production of, and consumption of biofuels.

Biofuel supply chains are adaptive systems as the agents in such systems adapt to other agents' actions and to changes in the environment[1]. Biofuel producers constantly change production patterns based on the demand for biofuels. Consumers of (bio)fuels adapt their consumption patterns based on the prices of biofuels and fossil fuel.

[1] Environment is defined as everything that lies outside of the object of the study (system). In modeling practice, the environment is defined as everything that influences the system but that it is not influenced by the system itself.

1.4.2. MODELING PARADIGM

At the core of this research is to understand the emergence of biofuel supply chains. Emergence is defined as *"the arising of novel and coherent structures, patterns, and properties through the interactions of multiple distributed elements"* [47]. This definition of emergence suggests that the modeling paradigm should have a generative and bottom-up capacity.

Approaches such as computational general equilibrium, supply chain optimization, and system dynamics are built on mathematical models based on a top-down paradigm and on an assumption of static system structure [48]. Thus, these tools are unsuitable for the exploration of the emergence of biofuel supply chains.

A promising approach for this research is agent-based modeling. Agent-based modeling (ABM) is a computational technique that describes a phenomenon in terms of unique and autonomous agents that interact with each other and their environment [37]. *"ABM combines the advantages of verbal descriptions, and analytical models"* [49]. That is, ABM allows a richer description of the problem without sacrificing the desirable rigor of formal analysis. Applications of agent-based modeling vary from economics [50, 51] and finance [52] to energy systems [53, 54], and supply chains design [40].

Agent-based modeling enables the modeling of complex adaptive systems, and thus the exploration of the phenomenon of emergence, because of four reasons. First, its bottom-up perspective positions the analysis from an actor-based perspective. Second, this actor-based perspective enables one to incorporate adaptation processes such as decision making into the analysis. Third, its capability to infer emergent system behavior from micro-level definitions. Finally, its adaptability enables the incorporation of different formalisms into the analysis.

1.5. SCOPE

IN this section, the scientific relevance and contribution of this dissertation are discussed.

1.5.1. SCIENTIFIC RELEVANCE

This is a multidisciplinary research that aims to understand the emergence of biofuel supply chains by bridging the gap between the school of Neo-institutional economics, complexity science, and computer science. The application of concepts from complexity science and Neo-institutional economics leads to a richer description of the phenomenon of the emergence of biofuel supply chains. This is of special interest to energy system modelers, for they can capture more of the phenomenon in the artificial system. The formalization of these concepts into a computational model enables one to carry out a rigorous analysis of the phenomenon. This is of special interest to the policymaker, for they can use the computational power to explore more possibilities and to assess which ones yield the best or most robust outcome.

1.5.2. CONTRIBUTION

This dissertation contributes to two different areas:

(Energy) policy analysis: optimization/equilibrium models are increasingly being used to assist in the analysis and design of policies supporting the expansion of the biofuel industry. These models, however, are unsuitable to explore the emergence of biofuel supply chains and are unable to incorporate realistic social processes into the analysis. This dissertation describes the development of a formal method to analyze the emergence of a biofuel supply chain. This method also enables one to include social processes into the analysis under more realistic assumptions (e.g. bounded rationality).

Energy system analysis and modeling: the dominant approach in the analysis of the energy systems is optimization. Thus, the use of models has been mainly focused on making predictions. The use of models to formalize and provide insights into the processes and mechanisms at work in the energy system is uncharted territory. This dissertation provides the conceptual and analytical tools to gain more insights into the workings of energy systems such as biofuel supply chains.

This dissertation is meant for the energy systems modeling community and policymakers alike. To the energy systems modeling community, this dissertation provides concepts and guiding principles for the agent-based modeling of biofuel supply chains. To policymakers, this dissertation provides insights into the workings of the German biodiesel supply chain, the Brazilian sugarcane-ethanol supply chain, and the Brazilian biojet fuel supply chain.

The main scientific contributions of this dissertation are the following:

Framework: the conceptual framework proposed offers an alternative for thinking about biofuel supply chains and describing agent-based models. The conceptual framework enables one to consider the introduction of social structures right from the conceptualization phase of the design of the agent-based model.

Methodological improvements in the agent-based modelling of biofuel supply chains: through the case studies, we illustrate how the conceptual framework underpins the modelling of social structures (e.g. spot market and contracts), policies (e.g. blending mandates, taxes, subsidies, and feed-in tariff), and actors behavior (e.g. decision making about production and consumption of biofuels).

Insights into the workings of existing biofuel supply chains: in the analysis of the German biodiesel supply chain, we showed that patterns in the expansion of production capacity can be explained by actors' investment decisions. It was hypothesized that these investment decisions are influenced by perceptions about market developments. We also found that in the event that an external shock (e.g. the introduction of a new policy) is introduced in the system, actors' adaptation mechanisms to changes in prices heavily influence the production of biodiesel.

In the analysis of the Brazilian sugarcane-ethanol supply chain, we found that doubling the production of ethanol by 2030 is feasible and that the expansion of the sugarcane processing capacity is driven most by a high gasoline tax (above 1.23 $R\$l^{-1}$). Fi-

nally, in exploring the emergence of a Brazilian biojet fuel supply chain from the existing sugarcane-ethanol supply chain, we found that this emergence hinges on the interaction of the feed-in tariff and the gasoline tax. In a tax-free gasoline regime, a feed-in tariff of 6 R$l^{-1} spurs the production of biojet fuel. Nevertheless, at higher levels of gasoline taxation (i.e. 2.46 R$l^{-1}), a feed-in tariff of 6 R$l^{-1} is insufficient to ensure the production of biojet fuel.

1.6. READER'S GUIDE

Chapter 2 describes the concepts that underpin the development of the conceptual framework for the analysis of a biofuel supply chain. This conceptual framework is to be used to guide the design of the agent-based model developed in the subsequent chapters.

Chapter 3 presents how this conceptual framework is used to guide the design of an agent-based model for the German biodiesel supply chain. This chapter also describes how the formalization of the conceptual framework into an agent-based model offers a means of explanation. With the help of the simulation model, we test the hypothesis that patterns in biodiesel production and production capacity result from investors' perception of market development.

Chapter 4 describes how the agent-based model underpins the analysis of the German biodiesel supply chain. This analysis includes the effect of the timing of the intervention of the policy, the effect of the interaction of biofuel policies, and the effect of actors' behavior on the development of the German biofuel supply chain.

Chapter 5 presents how the conceptual framework is used to guide the design of an agent-based model for the Brazilian sugarcane-ethanol supply chain. This chapter also presents how the agent-based model is used to explore the effect of different policy instrument such taxes levied on gasoline, hydrous and anhydrous ethanol, and the blend mandate on the evolution of the Brazilian ethanol supply chain.

Chapter 6 describes how the Brazilian ethanol supply may be a substrate for the emergence of a biojet fuel supply chain. In Chapter 7, we conclude by reflecting on our findings, discussing the contributions, and giving directions for further research.

The focus of study on Chapter 3 and Chapter 4 is on both understanding past developments and simulate (and to a certain extent replicate) trends of a historical biofuel supply chain, whereas the focus of study on Chapter 5 and Chapter 6 is on exploring future scenarios for the emergence of new supply chains.

2

CONCEPTUAL FRAMEWORK

Let a thousand flowers bloom,
a hundred schools of thought contend.

The goal of all theory is to make the basic elements as simple and as few as possible without having to surrender the adequate representation of experience.

Albert Einstein

The ideas of economists and political philosophers, both when they are right and when they are wrong, are more powerful than is commonly understood. Indeed the world is ruled by little else. Practical men, who believe themselves to be quite exempt from any intellectual influence, are usually the slaves of some defunct economist.

John M. Keynes, *The general theory of employment, interest, and money*

My conceptual framework, which basically emphasizes the importance of misconceptions, makes me extremely critical of my own decisions. I know that I am bound to be wrong, and therefore am more likely to correct my own mistakes

George Soros

2.1. INTRODUCTION

ONe of the main tenets of this dissertation is that a biofuel supply chain is a socio-technical construct. That is, the emergence and development of biofuel supply chains is shaped by actors' behavior and their interactions, the rules that govern these interactions, and laws of nature that govern the behavior of the physical elements.

As social reality admits a wide range of possibilities, it is difficult to find one framework or theory that provides a comprehensive description of a socio-technical system. To address this issue, we review and select a set of frameworks and theories that in combination allow us to explore the emergent behavior of socio-technical systems by describing the key concepts and the relationships between them.

The goal of this chapter is to describe both the theoretical underpinnings and the modeling approach used in this research. In this description, we distinguish three levels of theoretical analysis: frameworks, theories, and models [55]. In Section 2.2 and Section 2.3, we describe the frameworks and theories, respectively that ground the development of the conceptual framework. Then, this framework is described in Section 2.4. Finally in Section 2.5, we present an overview of the modeling paradigms that could be used to formalize the conceptual framework.

2.2. FRAMEWORKS

IN this section, we present two frameworks that base their ideas on the (Neo-) institutional economics school of thought.

2.2.1. MODELING AGENT SYSTEMS BASED ON INSTITUTIONAL ANALYSIS (MAIA) FRAMEWORK

MAIA is a formalization of the Institutional Analysis and Development framework (IAD) and extends it with theories such as the structuration theory [56] and social mechanism theory [57], and frameworks such as the Actor-centred Institutionalism (ACI) framework [58]. The IAD framework was developed by the Nobel laureate Elinor Ostrom with the aim of explaining and predicting outcomes in the management of common resources [59]. This framework provides a detailed structure for modeling institutions [60].

Modeling Agent system based on Institutional Analysis (MAIA) can be used as a meta-model[1] or as a framework according to the purpose. Meta-models aim to describe computational models whereas frameworks can be used for different purposes. In this dissertation, we use MAIA as a framework to facilitate the development of agent-based models that allow a richer description of the system.

The aim of MAIA is twofold. Firstly, to enable participatory model development by bringing agent-based modeling to policy analysts and social scientists, thereby allowing the introduction of problem domain insights into models. Secondly, to enable the incorporation of social concepts into agent-based models [62].

MAIA consists of five structures[2]:

[1] A meta-model is *"a formal description of a set of concepts that is used to describe a model and its properties"* [61]

[2] For a comprehensive description of the MAIA framework the reader is referred to [61]

- Collective structure: this structure specifies the actors (agents) in terms of attributes such as: name, property, personal value, information, physical component, possible role, intrinsic behavior, and decision making criterion.
- Constitutional structure: this structure describes the institutional environment which the agents are embedded in. Institutions are described by using the ADICO grammar of institutions. The acronym ADICO refers to the elements that make up an institutional statement: **A**ttributes (roles), **D**eontic (prohibition, obligation, permission), a**I**m (outcome), **C**ondition for the institution to hold, and the consequence ("**O**r else").
- Physical structure: this structure specifies the physical components of the system by defining the physical components (properties, behavior, type), the physical composition (components, composite), and the physical connection (properties, begin node, end node).
- Operational structure: this structure describes the narrative that shapes the dynamics of the system. Namely, it describes the actions of the agents and objects of the system and the order in which these actions are executed. The narrative is expressed in terms of the concepts of action arena, action situation, entity actions, and plan. Action arena can be defined as the place where individuals interact. Action situation represents a situation where agents interact with either other agents, with objects, or with the environment. A plan specifies the order of entity actions in an action situation. Finally, entity actions are the functions that run during one action situation.
- Evaluative structure: this structure specifies the set of independent and dependent variables proposed either to answer the modeling question or to validate the model or both.

2.2.2. INSTITUTIONAL ANALYSIS FRAMEWORK

The four levels of institutional analysis was developed by the Nobel laureate Oliver Williamson [63]. In this model, Williamson describes four levels of social analysis (see Figure 2.1). The top level corresponds to the culture of the society. That is, concepts such as norms, customs, religion, and traditions are located at this level. This level of analysis is taken as given by most economists as it changes very slowly (in the order of centuries or millennial).

The second level of analysis, the institutional environment, describes the rules of the game within which economic activity is organized. Formal rules such as constitutions, laws, and property rights are featured at this level of analysis. Although major changes in the rules of the game may be changed abruptly due to civil wars, military coups, and financial crises, institutions at this level usually undergo major changes in the order of decades or centuries.

The third level of analysis, governance, describes how the game is played. Namely, this level of analysis specifies how the economic actors organize themselves so as to reduce the transaction costs in their interactions. Institutions of governance undergo major changes in the order of a year to decade. Finally, the fourth level of analysis describes

how economic actors respond to changing market conditions by optimizing the allocation of resources. Institutions at this level are continuously changing.

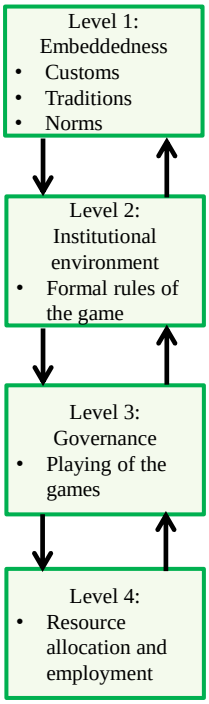

Figure 2.1: The four levels of institutional analysis framework. Adapted from [63]

2.3. THEORIES

THis section describes the theories that underpin the development of the conceptual framework proposed herein.

2.3.1. COMPLEX ADAPTIVE SYSTEMS THEORY

Complex adaptive systems (also known as complexity theory) is an umbrella of theories that seeks to understand the laws and mechanisms by which complex, coherent behavior emerges in a system. In the literature there are different definitions of complex adaptive systems [46, 64]. In this study, we adhere to the definition given by John Holland who defines a complex adaptive system as: *"[...] a dynamic network of many agents (which may represent cells, species, individuals, firms, nations) acting in parallel, constantly acting and reacting to what the other agents are doing. The control of a complex adaptive system tends to be highly dispersed and decentralised. If there is to be any coherent behaviour in the system, it has to arise from competition and cooperation among the agents themselves. The overall behaviour of the system is the result of a huge number of decisions*

made every moment by many individual agents"[46].

Complex adaptive systems have the following properties:

- Emergent behavior: it is the system behavior that arises from both the interaction of the system's individual components and their adaptation to each other and their environment [37].
- Adaptiveness: it is the *"ability of the components of the system of changing their behavior as a result of their interactions with other components and the environment"* [65].
- Self-organization: it is *"the process by which a system develops a structure or pattern without the imposition of structure from a central or outside authority, or when a system displays a different output as a result of internal processes"* [48].
- Path-dependence: the path of previous states, actions, or decisions determines the current and future states and decisions in a complex system [66]. That is, history matters
- Chaos: the behavior of the system is extremely sensitive to the initial parameter conditions [48].
- Non-linearity: the outputs are not proportional to their inputs.
- Observer-dependency: system's decomposition is dependent on system's observer. The observer chooses the perspective at which the system is observed [48].
- Agent-diversity: agents' attributes may differ from agent to agent [67].
- Intractability: it defines the impossibility of the exact prediction of an evolutionary process [68].
- Co-evolution: Nothing evolves in isolation. Entities in one subsystem continuously adapt to changes in the entities of a second subsystem, followed by the adaptation of the entities of the second subsystem to the change in the first [69].

2.3.2. SOCIO-TECHNICAL SYSTEMS THEORY

Socio-technical systems theory describes the relations of technologies and organizational forms in different settings [70]. As an object of analysis, a socio-technical system describes a system in terms of social network(s) and physical network(s) (see Figure 2.2) [71]. The system behavior emerges from the interaction of these networks. The social network consists of actors and the physical network consists of technical elements. An actor can be defined as an active social entity in the real world that makes decisions and performs a role. Examples of technical elements are the infrastructure, technology, software, etc.

The network of actors is governed by intentional relationships (e.g. customs, traditions, codes of conduct, legislation, property rights), whereas the physical system follows causal relationships (e.g. Newton's laws, Faraday's law of induction, Einstein's theory of relativity). Both types of relationships shape the behavior of the socio-technical system [72].

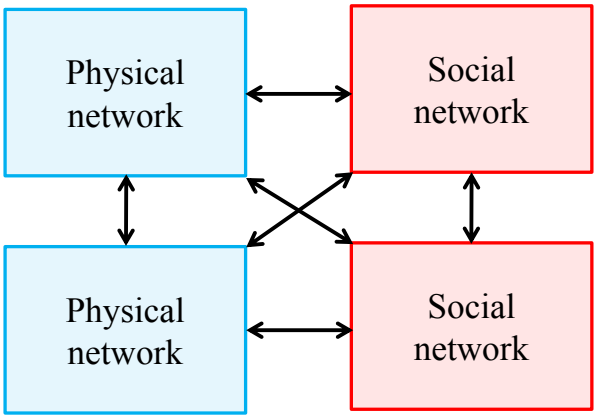

Figure 2.2: Description of a socio-technical system. Adapted from [71]

2.4. CONCEPTUAL FRAMEWORK

Concepts from the four levels of institutional analysis and socio-technical systems theory constitute the building blocks of the conceptual framework developed herein. These building blocks are: institutions, network of actors, and the physical system (see Figure 2.3). *"Institutions are the rules of the game in a society or, more formally, are the humanly devised constraints that shape human interaction. In consequence they structure incentives in human exchange, whether political, social, or economic"* [73]. Actors (individuals, organizations, firms, etc.) are the entities who make decisions and participate in a process by performing a role. The physical system refers to all physical elements in the system (infrastructure, technologies, artifacts, and resources).

Based on the complex adaptive systems theory, the conceptual framework distinguishes two levels of behavior: the micro-level and the macro-level. The behavior at the macro-level is the aggregate result of the interactions among and within the physical system, network of actors, and institutions (red dotted line in Figure 2.3). The behavior at the micro-level refers to attributes such as the states, rules, and actions performed by those elements. Emergent behavior can take place at both the macro-level and the micro-level. At the macro-level, emergent behavior is equivalent to the macro-behavior. At the micro-level, emergent behavior can occur in any of the building blocks (i.e. physical system, network of actors, and institutions) because of the interactions within these elements. To simplify the analysis, however, we only considered the emergence at the macro level. The framework also describes the co-evolution of the micro and macro behavior: *"behavior creates patterns; and pattern in turn influences behavior"* [74]. The black dotted line represents the system boundaries.

The MAIA framework is used to conceptualize these attributes. Namely, the collective structure is used to describe actors' decision making criterion and state variables such as personal values, roles, and intrinsic behavior; the physical structure is used to describe physical elements' state variables and behavior; the constitutional structure is used to describe institutions by using the ADICO grammar of institutions [60].

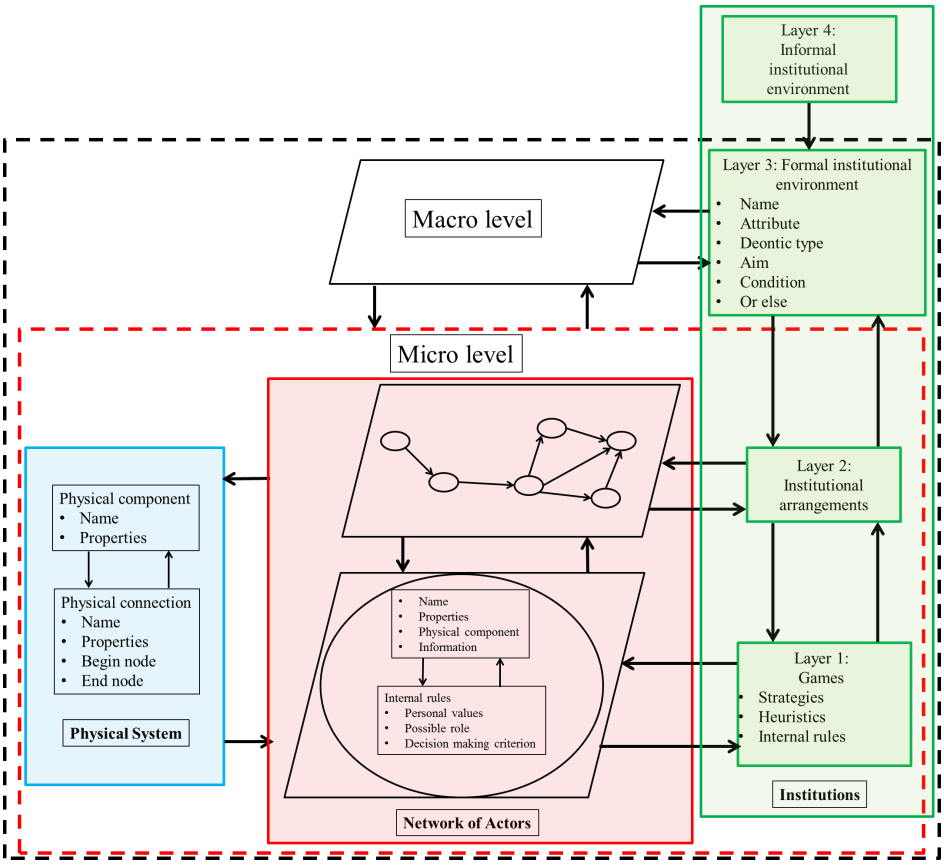

Figure 2.3: Conceptual framework

The four layer model is used to distinguish different levels of institutions: informal institutions, formal institutions, institutional arrangements, and resource allocation and employment. Nevertheless, the scope of the latter level of institutions is modified to account for actors' strategies and thus is called *games* [75]. This differentiation of institutions in different layers enables one to describe how institutions interact with the network of actors and with the behavior of the system at the micro and macro level. Likewise, the network of actors is divided in two scales to illustrate the interaction of institutions and actors at different levels (actor level, network level).

Layer 1, games, refers to the rules, norms and shared strategies that influence the behavior of individuals and shape the interaction between individuals within an organization. The level of institutional arrangements (governance structures) describes the different mechanisms of interaction (e.g. spot market, bilateral contracts, vertical integration) between and designed by actors to coordinate specific transactions. The formal institutional environment sets the rules of the game (e.g. tax exemptions, subsidies,

blending mandates, carbon tax). Finally, the informal institutional environment refers to culture. Norms, customs, traditions, and religion play a large role in this level. This institutional layer is assumed to be out of the system boundaries as it changes very slowly.

Unlike the interaction between institutions and the network of actors, the interaction between the physical system and the network of actors is less abstract. Actors design, build, operate, and invest in different elements of the physical system. In turn, the physical system enables actors to create wealth, to coordinate transactions, and to track compliance with certain laws and regulations.

By and large, the conceptual framework enables one to describe a system and its behavior in terms of its elements (physical system, network of actors, and institutions) and their interactions. Nevertheless, to shed some light on how these interactions bring about system behavior, one needs to formalize the framework into a computational model. The next section discusses how modeling paradigms can capture the main characteristics of the conceptual framework.

2.5. MODELS

THe formalization of the conceptual framework calls for a modeling paradigm that enables the description of complex systems. Namely, paradigms that account for the description of the framework's components (actors, physical system, and institutions) and their interactions. Modeling paradigms such as general/partial equilibrium models and optimization models enable one to describe the physical system and to a certain extent actors and institutions. These models, however, are unable to account for both the actors' interactions and the institutions that govern those interactions.

Modeling paradigms such as system dynamics (SD), discrete-event simulation (DES), and agent-based modeling (ABM) are suitable to simulate complex systems. These paradigms rest on different key assumptions and different building blocks to describe the system. Table 2.1 presents the main characteristics of the three simulation paradigms.

Table 2.1: Main characteristics of modeling paradigms for complex systems. Adapted from [65]

System Dynamics (SD)	Discrete-Event-Simulation (DES)	Agent-Based Modeling (ABM)
System oriented	Process oriented	Agent oriented
Homogenized entities	Heterogeneous entities	Heterogeneous entities
No representation of micro-level entities	Micro-level entities are passive objects that move through a system in a pre-specified process	Micro-level agents are active entities that can sense changes in the environment, interact with others and make autonomous decisions
Driver for dynamic behavior of system is "feedback loops"	Driver for dynamic behavior of system is "event occurrence"	Driver for the dynamic behavior of the system is agents decision and interactions
Formalization: stocks and flows	Formalization: Event, activity, and process	Formalization: agents and environment
continuous	discrete	discrete
System structure is fixed	Process is fixed	System structure evolves

These modeling paradigms differ in terms of approach (system oriented, process oriented, agent oriented), characteristics of the entities (homogeneous, heterogeneous), driver for system behavior (feedback loops, event occurrence, agents' decisions and in-

teractions), formalization (stock and flow; event, activity and process; agents and environment), and structure (system structure fixed, process is fixed, system structure not fixed).

An adequate formalization of the conceptual framework requires the capacity of describing entities with different characteristics. For instance, one finds that actors in the supply chain have different characteristics in terms of decision-making rules and attributes. Namely, farmers may differentiate with respect to the extent of arable land and biofuel producers with respect to the volume of production capacity. Unlike SD, DES and ABM are able to model heterogeneous entities. Hence, SD is an inadequate modeling paradigm to formalize the conceptual framework.

The actors described in the conceptual framework are active entities that are continuously adapting to changes in the behavior of other entities or changes in the environment or both. For instance, in the analysis of biofuel supply chains, one finds that actors in the supply chain make decisions about production or consumption of biofuels in response to actors demanding biofuel or in response to changes in fossil fuel prices. In this regard, ABM is more suitable than DES as ABM uses as a building blocks entities that can make sense of the environment, interact with other entities and make autonomous decisions. Conversely, DES features passive objects that move through a system in a prespecified process with no decision making capability and thus no capability of adaptation. Finally, and more importantly, ABM enables one to observe and explore emergent behavior because of its capability to infer emergent system behavior from micro-level definitions. From these arguments follows that agent-based modeling is the only suitable modeling paradigm to formalize the conceptual framework.

3

MODELING THE GERMAN BIODIESEL SUPPLY CHAIN

Essentially, all models are wrong,
but some are useful

George Box, *Empirical model-building and response surfaces*

. . . In that Empire, the Art of Cartography attained such Perfection that the map of a single Province occupied the entirety of a City, and the map of the Empire, the entirety of a Province. In time, those Unconscionable Maps no longer satisfied, and the Cartographers Guilds struck a Map of the Empire whose size was that of the Empire, and which coincided point for point with it. The following Generations, who were not so fond of the Study of Cartography as their Forebears had been, saw that that vast map was Useless, and not without some Pitilessness was it, that they delivered it up to the Inclemencies of Sun and Winters.

Jorge Luis Borges and Adolfo Bioy Casares, *On Exactitude in Science*

This chapter has been published as Moncada, J.A., *et al.*, A conceptual framework for the analysis of the effect of institutions on biofuel supply chains. Applied Energy, 2017. 185: p. 895-915.

The economic performance of biofuels supply chains depends on the interaction of technical characteristics as technological pathways and logistics, and social structures as actor behavior, their interactions and institutions. Traditional approaches focus on the technical problems only. Little attention has been paid to the institutional analysis of biofuel supply chains. This chapter aims to extend the analysis of the effect of institutions on the emergence of biofuel supply chains by developing a conceptual framework that combines elements of complex adaptive systems, (neo) institutional economics and socio-technical systems theory. These elements were formalized into an agent-based model. The proposed method is illustrated by a case study on a biodiesel supply chain in Germany. It was found that the patterns in production capacity result from investors basing their decisions on optimistic perceptions of the market development that increase with a favorable institutional framework. Conversely, patterns in biodiesel production cannot be completely explained by this mechanism. The proposed framework assisted the model conceptualization phase and allowed the incorporation of social structures into the agent-based model. This approach could be developed further to provide insights on the effect of different future deployment strategies on bioenergy systems emergence and development.

3.1. INTRODUCTION

THE depletion of fossil fuels, growing concerns about energy security and global climate change have led to growing worldwide interests in biofuels [18]. In fact, the substitution of fossil fuels with biofuels has been proposed by the European Union (EU) as part of a strategy to reduce greenhouse gas emissions from road transport, enhance energy supply and support development of rural communities [76].

One of the fundamental barriers to the establishment and development of biofuels supply chains is related to economics. Biofuels are not cost competitive with their fossil fuel counterparts and thus they need governmental intervention. Formal institutions such as mandatory blending targets, tax exemptions, subsidies and import tariffs are some of the government interventions widely used to stimulate production and increase consumption of biofuels around the world [18].

The economic performance of biofuels supply chains depends on the interaction of technical characteristics (technological pathways and logistics) and social structures (institutions and actors behavior). Technological learning mechanisms such as learning-by-searching and economies of scale depend on investment in research and development as well as on production capacity by financial actors (public or private). In turn, the decision to invest depends on the institutional framework. A stable and supportive institutional framework might reduce actors' risk perceptions and thus increase investment.

The scientific literature has been mainly focused on the technology [19, 77, 78], logistic [79, 80], and availability of feedstocks [81, 82] or some combination of them [21, 83]. In general, these studies leave aside the institutional framework and make normative assumptions on actors' behavior (*homo economicus*), or where the institutional framework is included, the focus is limited to formal institutions [27, 84].

The influence of institutions on the economic performance of biofuel supply chains is not only limited to the use of policy instruments. Institutions such as governance structures have proven to be an important barrier in the deployment of biofuels supply chains [85–87]. The selection of governance structure is crucial to competing on transaction costs. Similarly, the selection of technology is also pivotal to competing on production costs [28]. Indeed, the economic performance of a biofuel supply chain is the result of the interaction among technology, policy and management.

The interaction among institutions, actors' behavior and technical elements make the supply chain in general, and the biofuel supply chain in particular a complex adaptive system [1]. This inherent complexity calls for a multi-disciplinary approach and comprehensive conceptual analysis framework. To the best knowledge of the authors, a conceptual framework that encompasses institutional, technical and social elements in the analysis of the emergence of biofuel supply chains is still missing.

This paper proposes a conceptual framework combining elements of complex adaptive systems, (neo) institutional economics and socio-technical systems theory. To gain an understanding of the effect of policy on actor and system behavior, the conceptual

[1] Complex adaptive systems (CAS) refer to those systems whose overall behavior is intractable even when their components are very simple. The system behavior emerges as a result of the interactions between and adaptation of the individual components. Examples of such systems are: ecologies, immune systems, the brain, and economies [88]

framework is formalized into an agent-based model. The proposed method is illustrated by a case study on a biodiesel supply chain in Germany. The German biodiesel supply chain was selected as a study case as it has been one of the most important biofuels market in the world.

The major novelties of this work can be summarized as follows:

- Conceptualization of the interaction between technical elements and social elements (actors and institutions) and its effect on biofuels supply chains behavior.
- Model formalization by using an agent-based model approach.
- Incorporation of social structures into the agent-based model.

3.1.1. LITERATURE REVIEW

The study of the effect of institutions on biofuel supply chains has broadly been addressed by two different approaches: Analytical models and verbal descriptions. Analytical models rest on assumptions based on tractability considerations. Nuñez *et al.* [89] developed a mathematical model to analyze the impacts of biofuel mandates and trade distortions on land use, agricultural and transportation fuel markets, in the U.S and Brazil. The authors argued that benefits are bigger with free trade in biofuels and with the absence of distorting tax credits. Hoefnagels *et al.* [90] assessed the role of biomass and international trade for bioenergy in the EU27 under different renewable energy support scenarios. The authors argued that domestic biomass resources will remain the largest source of bioenergy, although increasing amounts of solid biomass will be traded in 2020. Wang *et al.* [91] investigated how the RIN mechanism influences the performance of the biofuel supply chain. They found that when a monopoly exists, a rigid mandate on blenders may decrease biofuel production. As these studies have focused on the study of the equilibrium, they have made coherent forecast and policy recommendations. However, besides that that optimality applies only in a limited context, they do not shed light on the mechanisms that lead to the formation of the equilibrium [74].

The second approach, verbal descriptions, are based on empirical or theoretical convincing arguments [49]. This flexibility to choose assumptions comes with a trade-off. Compared with analytical models, verbal models lack precision and rigor. Genus and Mafakheri used a neo-institutional approach to analyze bioenergy and sustainable energy systems in the UK [92]. The strategic niche management (SNM) framework has been used to explain the reason for the complicated development of biofuels in the EU [93]; to provide guidelines for the development of policies for stimulating biofuels [94]; and to provide insights for the emergence of a new biofuel supply chain [95].

Kaup & Selbmann [96] used a discourse coalition approach to explain the emergence of the German biodiesel industry as a result of national and supranational market interventions. Bomb *et al.* [97] analyzed the socio-political context of the biofuels industry in Germany and found that the institutional infrastructure played an important role in the emergence of the German biofuel industry. These studies have focused on how the institutional framework has influenced the evolution of the German bioenergy system. However, it is not well understood how to increase the performance of the system through institutional design.

These issues could be addressed by using Agent-Based Modelling (ABM), as *"ABM combines the advantages of verbal descriptions, and analytical models"* [49]. ABMs are powerful models that represent *"spatially distributed systems of heterogeneous autonomous actors with bounded information and computing capacity who interact locally"* [98]. Applications of ABMs vary from economics [50, 99, 100] and finance [51, 52] to food security, climate change [101, 102], energy systems [53, 103–105] and supply chains [106, 107]. ABMs are suitable to model complex adaptive systems due to their bottom-up perspective, adaptability and generative nature [67]. Moreover, ABM has been proven successful in the history-friendly[2] models formalization [109].

The idea of using ABMs to analyze (parts of) biofuel supply chains is not new. On the supply side, Happe *et al.* [43] investigated the impact of changes of policy regimes on farm structures using the agent-based model AgriPolis. The researchers found that the single area payment (SAP) had no significant effect on agricultural structure. On the demand side, Van Vliet *et al.* [39] developed an agent based model to analyze motorists' preferences based on real-world choice mechanisms. The authors concluded that a successful transition from fossil fuels to biofuels requires policy stability. Shastri *et al.* [42] analyzed the dynamics of the adaptation of Miscanthus as an agricultural crop and its impact on biorefinery capacity. The authors concluded that the production of feedstock depends not only on technological advances and economic mechanisms, but also on the behavioral aspects of the actors involved in the system. Alexander *et al.* [38] used an agent-based approach to model the UK perennial crop, including the interaction of supply and demand. They found that the limiting step in the rate of adoption of a new crop for a farmer is the spatial diffusion process. Singh *et al.* [40] addressed the problem of biorefinery supply chain network design under competitive feedstock markets by using an hybrid approach. An agent-based model was developed to simulate the feedstock markets and a mixed-integer nonlinear program was developed to design the supply chain network. The authors found that the competition for feedstock influences the profit of biorefineries and that such an impact should be taken into account when designing a biofuel supply chain. The literature shows that these models, unlike the optimization approach, recognize the importance of socio-economic and behavioral aspects of various stakeholders within the biofuel supply chain on the performance of the system. However, apart from the work of Happe *et al*, these studies did not analyze the effect of institutions on (parts of) biofuel supply chains development.

The remainder of this chapter is organized as follows. Section 3.2 provides background on the policy landscape in the biodiesel production in Germany. Section 3.3 describes the conceptual framework and the conceptualization of the agent-based model. It also describes the data used in the simulation, and the data used in its calibration, the uncertainty analysis, and the robustness analysis. Section 3.4 and Section 3.5 describe and discuss the results obtained, respectively. Conclusions are presented in Section 3.6.

[2] History friendly models *"are formal models which aim to capture – in stylized form – qualitative and appreciative theories about the mechanisms and factors affecting industry evolution, technological advance and institutional change put forth by empirical scholars of industrial economics, technological change, business organization and strategy, and other social scientists."* [108]

3.2. CASE STUDY

3.2.1. BIODIESEL PRODUCTION IN GERMANY AND POLICY LANDSCAPE

Production of biodiesel in Germany began in 1991, with rapeseed as the main feedstock. Biodiesel production grew exponentially from 1997 onwards. Whereas in 1998 German production capacity was 65000 t/y, by 2006 it had grown to 3.5 million t/y [96, 97]. Governmental interventions, such as introduction of standard certifications and a single payment scheme, and rising oil prices have contributed to this growth in German biodiesel production [110].

In 1992, the common agricultural policy (CAP) decommissioned a percentage of agricultural land to be set aside. The EU stipulated annually the set-aside land quota depending on the state of the market. The extension of the quota oscillated between 5% and 15% of the total agricultural area. Farmers were allowed to cultivate non-food crops on those set-aside lands without losing the subsidy granted by the EU. However, financial penalties were inflicted on farmers who tried to sell set-aside rapeseed on the food market. The set-aside is considered by Kaup & Selbmann [96] as the initial incentive that stimulated the development of the biodiesel industry. The taxation imposed on mineral oil based fuels enabled biodiesel to find a market and become an economically competitive fuel [110].

In 1999, ecological taxation became binding. The rationale was to shift the cost of greenhouse gas emissions (GHG) reduction to polluters (fossil fuels production companies). Biodiesel was exempted from this tax which improved its economic competitiveness compared to fossil diesel. This exemption, along with the high crude oil price in 1999, led to an increase in both biodiesel production and production capacity in the coming years.

In 2003 the EU adopted a fundamental reform of the CAP. To stimulate further liberalization of the EU agricultural market, production and volume focused policies were shifted to area related payments. The aim of this agricultural policy change was twofold: to base agricultural production on market forces and to harmonize prices of agricultural goods with world market levels [110, 111].

In 2004, biofuels were included in the mineral oil tax law and explicitly guaranteed tax exemption until the end of 2009. However, the EU commission stated a clause of an annual revision and the suspension of the tax privilege if overcompensation was found. In 2005, the crude oil prices reached an all-time high, leading to an overcompensation of biodiesel and a loss of its privileges.

The energy tax law came into force in 2006, replacing the mineral oil tax law. This policy defined an annual increase of the tax rate on biodiesel, which led to a decrease in demand. The biofuel quota law was introduced in 2007 to offset the negative impacts of the energy tax law and to keep stimulating the biodiesel industry. Biofuel producers and distributors are coerced to meet a biodiesel quota through a penalty. The biofuel policies introduced in 2006 and 2007 brought about a stagnation of biodiesel production and the shutdown of mostly small and middle sized biodiesel production facilities [96]. Biodiesel imports also increased during this period [112]. In 2008, the set aside land policy was abolished. The total amount of biodiesel produced in Germany in the period 2000-2011 was 20.86 million tons, saving approximately 2.49 million tons of CO2 equivalents on an annual basis, equaling 0.25% of the total German annual GHG emissions.

Increasing public skepticism (mainly from NGOs) towards the biofuel industry encouraged the German government to issue a draft for the biomass sustainability ordinance in 2007. With this mandatory ordinance, the government aimed to promote the production of specific GHG efficient biofuels. This new German legislation became effective in 2015. This new legislation has dramatically changed the rules of the game in the biodiesel arena as the price of biodiesel is based on the environmental performance of the production processes. Subsequently, biodiesel produced using environmental friendly technologies is worth more than that produced using technologies that are not efficient in mitigating GHG emissions [113].

3.3. THEORY AND METHODS

THE conceptual framework presented in this chapter builds on the elements described in the framework proposed by Williamson [63, 114] and modified posteriorly by Koppenjan & Groenewegen [75]; by Ghorbani [62] and by Ottens *et al.* [72].

As shown in Figure 3.1, the conceptual framework consists of three elements: institutions, network of actors, and the physical system. *"Institutions are the rules of the game in a society or, more formally, are the humanly devised constraints that shape human interaction. In consequence they structure incentives in human exchange, whether political, social, or economic"* [73]. Actors (individuals, organizations, firms, etc.) are the entities who make decisions and participate in a process by performing a role. The physical system refers to all physical elements in the system (infrastructure, technologies, artifacts, and resources). The behavior at the macro-level is the aggregate result of the interactions among the physical subsystem, network of actors, and institutions (red dotted line in Figure 3.1). The behavior at the micro-level refers to the states, rules, and actions performed by those elements. The co-evolution of the behavior at the micro and macro level is also incorporated in the framework: *"behavior creates patterns; and pattern in turn influences behavior"* [74]. The black dotted line represents the system boundaries.

Institutions are composed of four different layers, as institutions interact with the network of actors and with the behavior of the system at the micro and macro level. These layers are fully interconnected. Similarly, the network of actors is divided in two scales to illustrate the interaction of institutions and actors at different levels (actor level, network level).

Layer 1, games, refers to the rules, norms and shared strategies that influence the behavior of individuals and shape the interaction between individuals within an organization. The level of institutional arrangements (governance structures) describes the different mechanisms of interaction (e.g. spot market, bilateral contracts, vertical integration) between and designed by actors to coordinate specific transactions. The formal institutional environment sets the rules of the game. This layer is composed of the policy makers and government agents who strive to steer the macro behavior of the system to some desired state (e.g. economic growth, transition to low carbon economy, etc.). Finally, the informal institutional environment refers to culture. Norms, customs, traditions, and religion play a large role in this level. This institutional layer is assumed to be exogenous as it changes very slowly.

Unlike the interaction between institutions and network of actors, the interaction between the physical system and the network of actors is less abstract. Actors design, build,

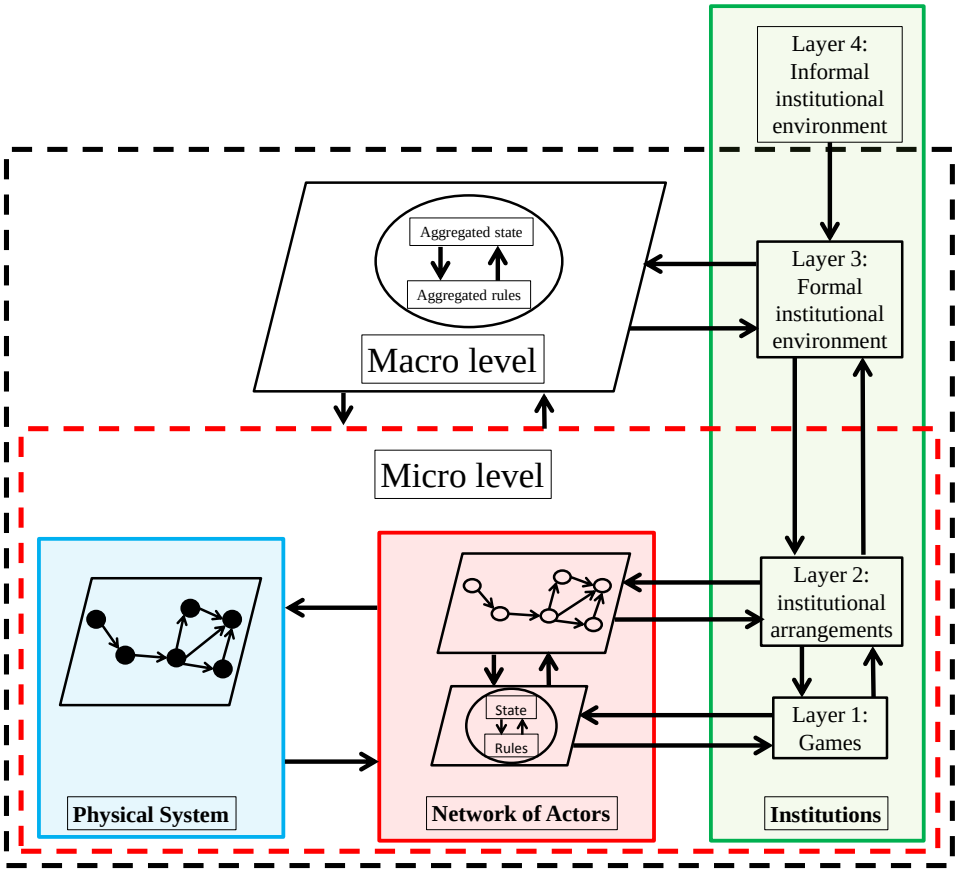

Figure 3.1: Conceptual framework[3]

operate, and invest in different elements of the physical system. In turn, the physical system enables actors to create wealth, to coordinate transactions, and to track compliance with certain laws and regulations.

Three theories underpin this conceptual framework. Firstly, complex adaptive systems (CAS) theory is used to explain the creation of the macro behavior of the system (emergence) as a consequence of the interaction among the different system elements (complexity) and how, in turn, these elements adapt to the macro behavior they created (adaptation). This interplay between the macro and the micro behavior of the system usually leads to self-organization. Secondly, (neo) institutional economic theory is used to specify the interaction between institutions and the network of actors and to describe the interaction between actors (spot market, bilateral contracts, vertical integration). Actors' properties such as learning, and bounded rationality come from this theory. Like CAS, (neo) institutional economics focuses on the concept of evolution rather than equi-

[3]This figure is not exhaustive. A subsystem that accounts for the ecosystems services could also be introduced.

librium. Finally, the theory of the critical price linkages and economics of blend mandates states that biofuel policies cause a link between crop and biofuel prices. Unlike the crop-biofuel price link, the biofuel-fossil fuel link is policy-regime dependent. If a biofuel consumption subsidy is enacted, biofuel prices, and therefore crop prices, are locked onto fossil fuel prices. When the mandate is binding, biofuel prices are delinked from fossil fuel prices.

Supported by these theories, the conceptual framework is further formalized into an agent-based model to analyze the influence of institutions on biofuel supply chains, with German biodiesel production as a case study.

3.3.1. DEVELOPMENT OF THE AGENT-BASED MODEL

The agent-based model for a biofuel supply chain is developed based on the methodology proposed by van Dam *et al.* [48]. The purpose of the model is to understand how biofuel production and production capacity could have evolved as a result of different agricultural and/or bioenergy policy interventions. The scope of the present work is limited to the description of the proposed conceptual framework and its formalization into an agent-based model. The findings of the model will be presented in further studies.

Key steps in the development of the model are problem formulation, system decomposition, and concept formalization. The conceptual framework presented in Figure 3.1 along with the MAIA framework [62] were used to decompose the system into relevant components. The physical system defines the physical components. Technical artifacts (production plants, and distribution centers); technologies (transesterification); resources (land), and products (rapeseed, rapeseed oil, and biodiesel) are part of it. This subsystem consists of two sub-classes: physical component and physical connection.

Physical component: It is an entity that can be used and/or owned by different roles in the system. A physical component has the following attributes:

- Name: Identifier of the object.
- Properties: Collection of parameters that define a physical component. Surface area, yield, production costs and marginal costs are the main properties of the entities used in the biodiesel system.

Physical connection: It links two physical components. A distribution pipeline to transport fuel is a good example of a physical connection. The physical connection has the following attributes: name, properties, begin node, and end node.

The network of actors consists of four agents: suppliers, producers and distributors. Agents are described by the following attributes:

- Name: Identifier of the agent.
- Properties: Collection of parameters that defines an agent.
- Personal values: Number of intentions of an agent that determine his decision-making behavior. Risk aversion and making profits are considered as a personal value for the supplier agents. Self-interest and making profits are considered as a personal value for producers and distributors.

- Information: the information available to an agent. The supplier agent knows the price of rapeseed and wheat in the market.
- Physical components: Agents can also possess physical components. Producers and distributors agents have biodiesel production plants, and distribution capacity, respectively.
- Roles: The potential roles the agent may take. Suppliers take the role of farmers, producers the role of biofuel producers, and distributors the role of biofuel distributors. Markets and government are considered external agents. An external agent does not take any role.
- Intrinsic behavior: The capabilities an agent has independent of the role he is taking. Although not incorporated in the model, an example of intrinsic behavior for the agents is aging.
- Decision making behavior: The criteria that the agent uses to choose between a set of options. Farmers have to decide how much energy crops to produce; biofuel producers and biofuel distributors need to decide whether to meet the quota or pay the penalty; or expand capacity. These decisions are based on profitability.

Two levels of institutions are included in the description of the German biodiesel supply chain. The layer of "actors and games" is omitted as it was already incorporated in the definition of the agents. The layer of institutional arrangements is defined by the attributes:

- Name: Identifier of the object.
- Type: Class of governance structure (spot market, bilateral contracts, and vertical integration).
- Actors: Specifies the agents in the transaction.

The organizational structure implemented in the model is the bilateral contract. However, the price of the rapeseed is assumed to be estimated based on (endogenous) market mechanisms. The demand curve for rapeseed is drawn based on the resources, preferences, and information of the biofuel producers. Each biofuel producer bids into the rapeseed market the amount of rapeseed and the price that he is willing to pay. An aggregated demand curve is then built with this information. The rapeseed price is determined based on the total amount of rapeseed bid by farmers in the market as shown in Figure 3.2.

Each biofuel producer estimates his own bids for rapeseed based on expectations as is shown in the following equation:

$$P_{r_j}^{bid} = A + B \tag{3.1}$$

Where:

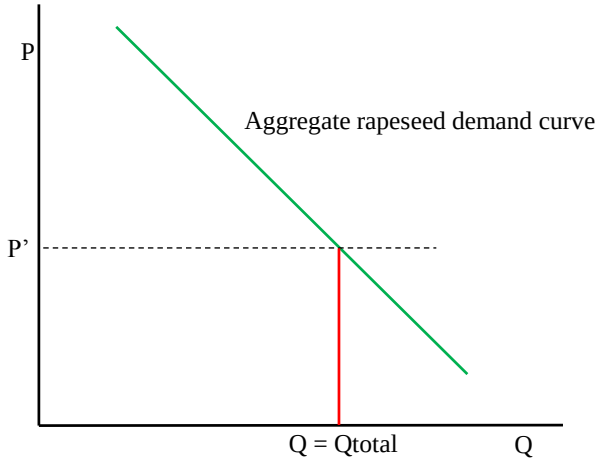

Figure 3.2: Hypothetical aggregated demand curve for rapeseed and rapeseed equilibrium price

$$\beta = \frac{Y_{o-b_j}}{Y_{r-o_j}} \tag{3.2}$$

$$\theta = \beta Y_{b-g_j} \tag{3.3}$$

$$\gamma = Y_{r-rm_j} \tag{3.4}$$

$$r = \frac{P_{rm}}{P_r} \tag{3.5}$$

$$A = \frac{\beta}{\left(1-\left(r\gamma\left(1-PM_j\right)\right)\right)}\left(P_{bp_j}^{exp}\left(1-PM_j\right)-c_{b_j}\right)\frac{1}{\rho_b} \tag{3.6}$$

$$B = \frac{\theta}{\left(1-\gamma\left(1-PM_j\right)\right)}\left(P_g\left(1-PM_j\right)\right) \tag{3.7}$$

The market for biodiesel is modelled according to the policy. If the tax (credit) is binding, then the demand curve for biodiesel is drawn based on the resources, preferences, and information of the distributors. Each distributor bids into the biodiesel market the amount of biodiesel and the price that he is willing to pay. Then, an aggregated demand curve is built with this information. The biodiesel (producer) price is determined based on the total amount of biodiesel bid by biofuel producers in the market as shown in Figure 3.3.

Each distributor bids into the biodiesel market based on expectations. As shown in Equation (3.8), it is assumed that the total production costs are equivalent to the costs of procuring biodiesel.

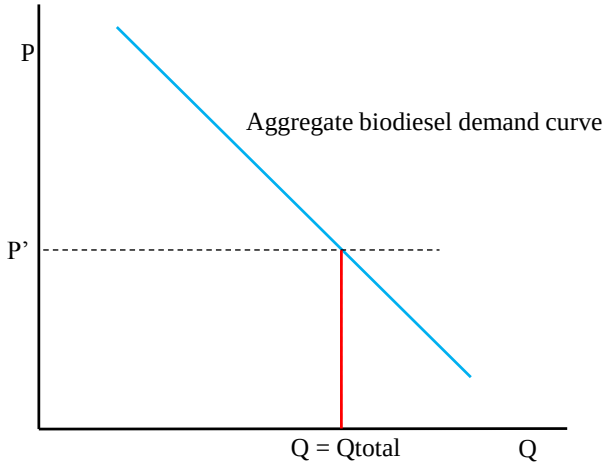

Figure 3.3: Hypothetical aggregated demand curve for biodiesel and producer price

$$P_{bp_k}^{bid} = P_{b_k}^{exp}\left(1 - PM_k\right) - t_b \tag{3.8}$$

On the other hand, when the mandate is binding the (producer) price for biodiesel is determined using the biofuel producers' supply curve and the mandate (quota) as is shown in Figure 3.4.

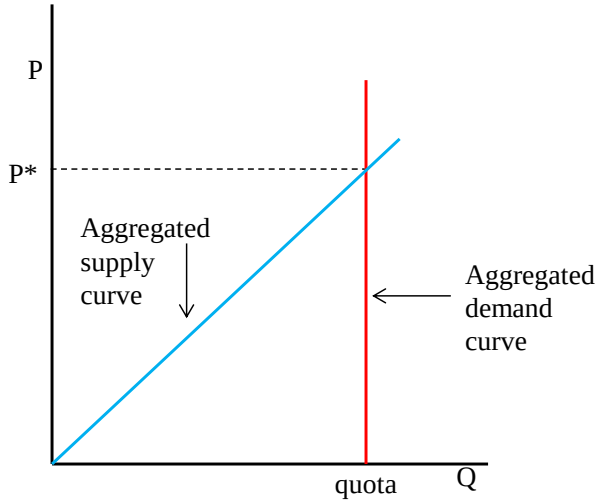

Figure 3.4: Hypothetical aggregated supply and demand curve for biodiesel when a mandate is imposed by the government

Biofuel producers estimate their own individual supply curves for biodiesel based on marginal cost.

$$MC_{b_j} = \frac{dTC_{b_j}}{dq_{b_j}} \tag{3.9}$$

Where:

$$TC_{b_j} = \left(C_{o_j} Cap_j\right) + \left(P_{r_j}^{exp} q_r\right) \tag{3.10}$$

The formal institutions are structured using the syntax of the grammar of institutions proposed by Crawford and Ostrom [60]. An institution has the following components (ADICO) [115]:

- ***A***ttributes: The roles that follow this institution.
- ***D***eontic type: An institution can be in the form of prohibition, obligation or permission.
- a***I***m: The action that agent should take when following this rule. Biofuel producers must pay tax if the energy tax is binding.
- ***C***ondition: the condition for this institution to take place.
- ***O***r else: The sanction for the agent taking the role if he does not follow this institution.
- Institutional type: Statements can be classified as: rules, norms, and shared strategies.

Table 3.1 presents the conceptualization of the institutions analyzed in this study. 'Agricultural reform' refers to the common agricultural policy (CAP) enacted in 1992. The 'liberalization of the EU agricultural market' indicates the fundamental reform of the CAP in 2003. The energy tax act specifies the energy tax law enacted in 2006. The biofuel quota act refers to the biofuel quota law introduced in 2007.

It was assumed that formal institutions are exogenous. Both policies, the agricultural reform and the liberalization of the agricultural market, impact farmers' decisions on crop allocation. The Biofuel Quota Act influences biofuel producers' decision making on rapeseed procurement. The Energy Tax Act affects the profitability of the biofuel producer. For a more detailed description of the physical and social components the reader is referred to [62]. An overview of the concept formalization is presented in Figure 3.5.

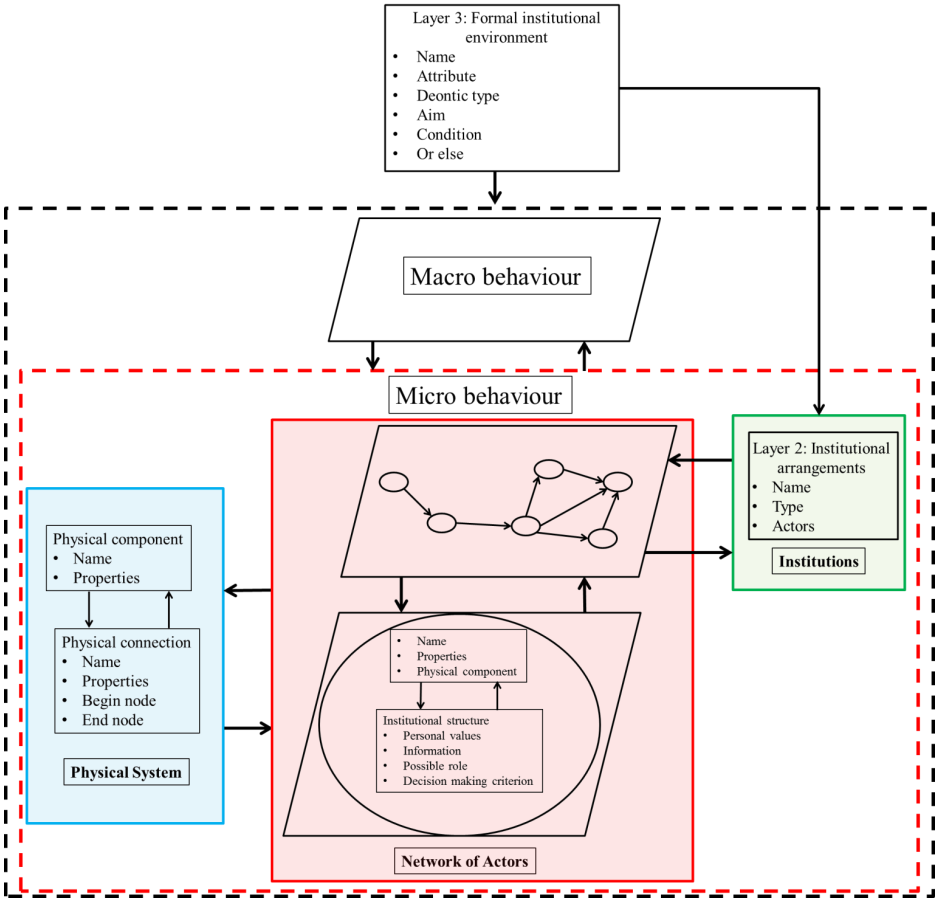

Figure 3.5: Concept formalization

Table 3.1: The institutional table for the biodiesel energy system

Institution						
Name	Attribute	Deontic type	Aim	Condition	Or else	Type
Agricultural reform	Farmer	must	sell crops to the energy market	If crops were grown in the set aside land	Fine selling	Rule [a]
Liberalization of the EU agricultural market	Farmer		sell crops to the energy market	If prices in the energy market are equal or high to those prices in the food market regardless of the land type		Shared strategy [b]
Energy Tax act	Biofuel producer	must	Pay tax	If energy tax is binding	Fine producing	Rule
Biofuel quota act	Biofuel producer	must	Produce the amount of biodiesel assigned to meet the demand	If biofuel quota is binding	Fine producing	Rule
	Biofuel distributor	must	Distribute the amount of biodiesel assigned to meet the demand	If biofuel quota is binding	Fine distributing	Rule

[a] Rule: it includes all the elements of the ADICO syntax. That is, “attribute”, “deontic type”, “aim”, “condition”, and “or else”
[b] Shared strategy: it includes all the elements of the ADICO syntax but “deontic type”, and “or else”

On an abstract level, a biofuel supply chain can be considered as a network of two co-evolutionary subsystems: technical and social systems. The elements identified in the system decomposition phase were structured as a network as presented in Figure 3.6. In the network, suppliers adopt the role of farmers, producers adopt the role of biofuel producers, and distributors adopt the role of biofuel distributors. Agents in the system interact between them, with other objects, and with the environment through different mechanisms: trading (bilateral contracts), ownership, and price signals, respectively. Farmers and biofuel producers trade rapeseed; biofuel distributors own distribution centers; and agents make decisions based on information provided by markets. The environment is composed of the government. The government can influence the price of the different products through incentives in the different markets.

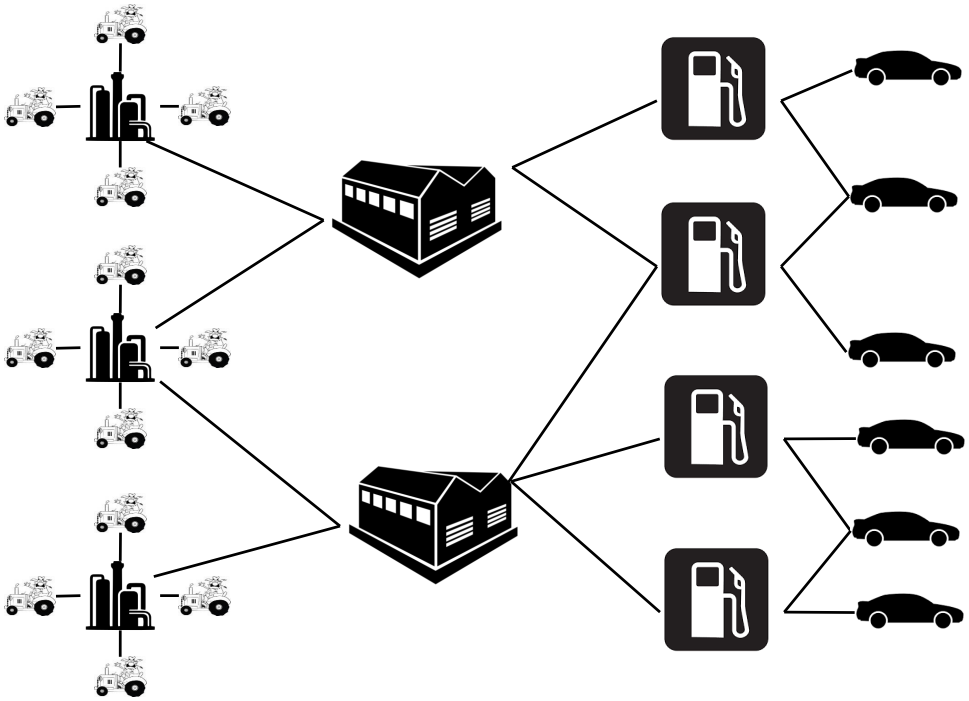

Figure 3.6: Representation of a biofuel supply chain.

3.3.2. MODEL NARRATIVE

An overview of the model narrative is presented in Figure 3.7. In line with the MAIA framework, the concepts expressed in this narrative are: action arena, action situation, plan, and action entity. Action arena can be defined as the place where individuals interact. Action situation represents a situation where agents interact with either other agents, with objects, or with the environment. A plan specifies the order of entity actions in an action situation. Finally, entity actions are the functions that run during one action situation.

During the first year of the simulation, the farmers make land allocation decisions for the energy crops based on speculation. Biofuel producers and distributors forecast producer and wholesale prices for biodiesel for the second year, respectively. They also estimate their own individual demand curves based on expectations. Then, the aggregated demand curve for rapeseed and biodiesel are built using individual demand curves. The market prices for rapeseed and wheat are determined based on aggregated demand curves and the actual production. Rapeseed is sourced by biofuel producers through their closest farmers. This procedure is repeated until the biofuel producer either fulfills his operating capacity, there is no more rapeseed available in the system, or it is too expensive to procure it. Farmers calculate the profit or loss associated with energy crop production. This information is then used to change the land allocation decisions in the subsequent years.

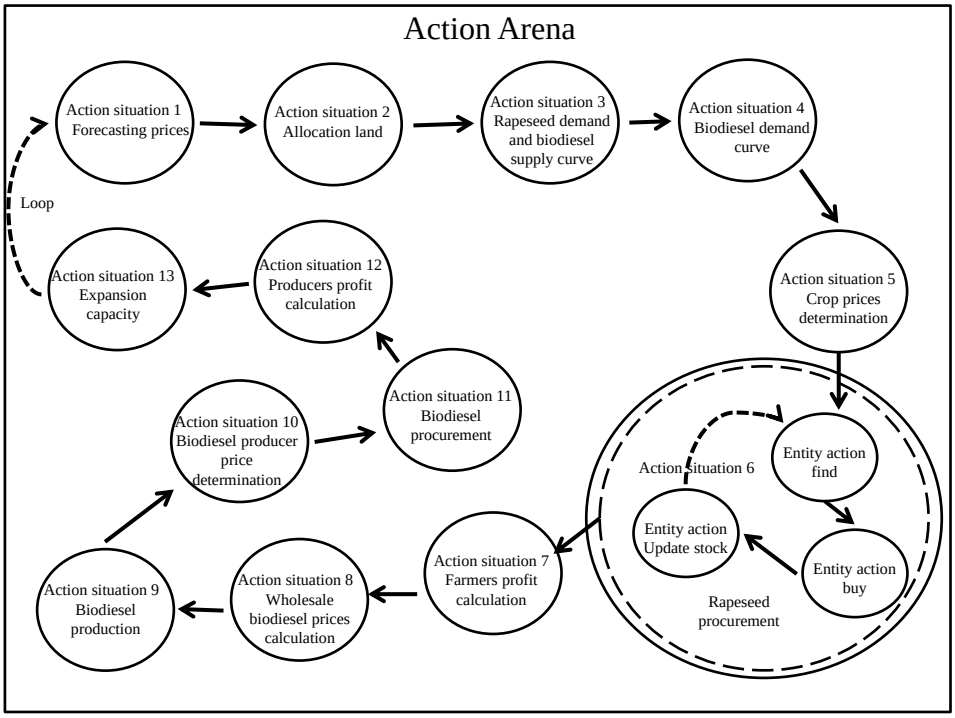

Figure 3.7: Model narrative expressed in terms of entity actions, action situations, and plan. An arrow shows a sequence. The dotted arrow represents a loop.

Biodiesel production starts in the second year. The market price for biodiesel (producer price) is determined based on the aggregate demand curve for biodiesel. Biodiesel is then procured by distributors through their closest biofuel producers. Although not shown in Figure 3.7, this action situation is executed similarly to the action situation *"rapeseed procurement"*. Biofuel producers decide whether to expand capacity (build a new plant) based on the availability of feedstock, the demand for the biofuel, and the net

present value. The number of plants to be built is influenced by producers' perception of market development.

As this cycle is repeated in the second year of production, cropland allocation decisions are modified based on the profitability information available and previous experience. Biofuel producers and distributors learn and adapt their method to forecast biodiesel producer price and wholesale price, respectively. New aggregated demand curves for rapeseed and biodiesel are determined from the modified individual demand curves.

The action situations sequentially take place in the action arena and they are repeated until the stop criteria (final year) are met. Agents adapt to the environment in each iteration. The adaptation mechanism is incorporated into *"forecasting prices"*. Agents improve their forecasting based on the following equation [116].

$$C_t^e = C_{t-1}^a \left(C_{t-1}^e\right)^{(1-a)} \tag{3.11}$$

Appendix A describes the algorithms used to model the decision making of farmers and biofuel producers.

The main model assumptions are summarized below:

- One tick is equivalent to one year. This time frame was selected based on the time scale to sow and harvest rapeseed.
- It is assumed that the biodiesel and rapeseed market in Germany is a closed system. Any interaction with world market forces is neglected as the model's purpose is to understand the influence of national policies on the emergence of the German biodiesel supply chain.
- Agents aim to maximize profits by using the limited information available to them. That is, agents are assumed to be profit maximizers with bounded rationality.
- When the liberalization of the market became binding, farmers sell all the rapeseed and wheat produced during the year. Any rapeseed left by biofuel producers is bought by the food sector. In practice, due to food security reasons, the food sector demand for rapeseed is first satisfied
- Distributors sell all the biodiesel procured in each year. This assumption was made to focus the analysis to the behavior of farmers and biofuel producers as the modeling question is directly related with behavior of these two agents.
- When acting as investors, all biofuel producers share the same perception on market developments. This perception is translated into the number of new plants to be built. Optimistic perceptions lead to more investment and thus to the construction of more plants. This parameter is assumed to be a function of the institutional framework, specifically of the biodiesel tax and the biodiesel quota institutions.

$$pmd = f(t_b, q_b) \tag{3.12}$$

Equation (3.12) is assumed to have the following properties:

– If the biodiesel tax is enacted, then the perception on biodiesel market development is neutral. In this case, the biofuel producer invests in a new plant if $NPV > 0$.

$$t_b \neq 0 \rightarrow pmd = 1 \tag{3.13}$$

– If the biodiesel tax is not enacted, then the perception on biodiesel market development is overly optimistic. In this case, the biofuel producer invests in new plants if $NPV > 0$.

$$t_b = 0 \rightarrow pmd > 1 \tag{3.14}$$

– If the biofuel quota is enacted, then the biodiesel market is considered adverse for investment. In this case, the biofuel producer does not invest in a new plant.

$$t_b = 0 \rightarrow pmd = 0 \tag{3.15}$$

- Wholesale biodiesel prices P_b are calculated based on kilometers equivalent liters of diesel. Biodiesel gets 0.913 km per liter compared to a liter of diesel [117].

$$P_b = \lambda P_d \tag{3.16}$$

3.3.3. DATA COLLECTION

Techno-economic parameters were retrieved from studies focusing on rapeseed and wheat production in Germany and studies focusing on biodiesel production using esterification as a chemical route. Table 3.2 presents the values for production cost and yields used in this study. As no technological-learning was assumed, the values of these parameters remain constant during the simulation. Appendix B presents the data used to carry out the techno-economic evaluation. Yields for rapeseed and wheat are those reported by the FAO [118]. These data are presented in Appendix C.

Values for subsidies given during the liberalization of the EU agricultural market are reported in Table 3.3. This includes premium agricultural land, premium grass land, standard agricultural land, and extra fee energy crops; and values for the biodiesel tax and penalty when the Energy Tax Act and Biofuel Quota Act came into force. The biodiesel production capacity constraint was calculated based on historical data. Table 3.4 presents the institutional chronogram.

Table 3.5 presents the distance variable transportation cost of rapeseed and biodiesel. The transportation cost is calculated with the following equation:

$$tc_b = tc_p l_c L \tag{3.17}$$

Table 3.2: Techno-economic parameters

Parameter	Value	Unit	Reference
Rapeseed production cost	240 - 278	$€\,t^{-1}$	Parkhomenko [119]
Wheat production cost	80-130	$€\,t^{-1}$	Kleinhanss et al. [120]
Biodiesel fixed production cost	0.08 – 0.11	$€\,l^{-1}$	Charles et al. [121]
Yield rapeseed oil[a]	0.4 (0.05)	$kg_{oil}\,kg^{-1}_{rapeseed}$	Berghout [110]
Yield biodiesel[a]	0.97 (0.05)	$kg_{biodiesel}\,kg^{-1}_{oil}$	Berghout [110]
Yield glycerol	0.11	$kg_{glycerol}\,kg^{-1}_{biodiesel}$	Berghout [110]
Yield rapeseed meal	0.56	$kg_{rapemeal}\,kg^{-1}_{rapeseed}$	Berghout [110]

[a] Normal distribution X (Y); X = mean; Y = standard deviation

Table 3.3: Policy parameters

Parameter	Value	Unit	Reference
Standard agricultural premium	301	$€\,ha^{-1}$	Arnold et al. [122]
Extra fee energy crops	45	$€\,ha^{-1}$	Arnold et al. [122]
Tax biodiesel	0.3	$€\,l^{-1}$	Berghout [110]
Penalty biodiesel	0.5	$€\,l^{-1}$	Berghout [110]
Ratio quota/total capacity[a]	0.65	–	Kaup and Selbmann [96]

[a] The ratio total capacity is calculated using historical data from Kaup and Selbmann [96]

Table 3.4: Institutional chronogram

Institution	Period
Agricultural reform	1992 - 2002
Liberalization of the EU agricultural market	2003 - 2014
Energy Tax act	2006 - 2014
Biofuel quota act	2007 - 2014

The conversion factor was calculated based on the longest distance in Germany (North to South, 853 km). Assuming that Germany is a square with 800 km length, each patch in the agent based model has a length of 25 km. This value was used; $l_c = 25\,\text{km}$.

Table 3.5: Logistic parameters

Parameter	Value	Unit	Reference
Rapeseed transportation cost	0.05	$€\,t^{-1}\,km^{-1}$	You et al [123]
Biodiesel transportation cost	5,00E-05	$€\,l^{-1}\,km^{-1}$	Own calculations

The values of the socio-economic parameters assumed in this study are reported in Table 3.6 and Table 3.7. It is assumed that when biofuel producers procure rapeseed from farmers in surrounding areas (within their *"vision"*) the transportation costs are not account for. The same assumption also applies to the interaction between biodiesel distributors and producers. As it is shown in Table 3.2, Table 3.6, and Table 3.7, random variation was introduced in some elements to add an element of heterogeneity.

The model was developed using an object-oriented approach in NetLogo [124]. Each agent type (farmer, biodiesel producer and distributor) is declared as an object class with a set of attributes that are common to each member of the class. Properties such as land and capacity are allocated to the agents based on their yields. Higher yields lead to a higher land size or capacity volume. This allocation criterion aims to mimic economies of scale in the system. Yields are allocated randomly.

3.3.4. CALIBRATION OF THE MODEL

The model was calibrated using the strategy proposed by Railsback and Grimm [37]. Initially, three parameters were chosen as candidates to calibrate the model: the initial fraction of arable land to be used to produce the energy crop, blc, the rate of land conversion, rlc, and the biofuel producer's perception of the biodiesel market development, pmd.

The rationale for the selection of these parameters is that they exhibit high uncertainty in their values in comparison to techno-economic, logistic, and policy instrument parameters. To reduce the amount of parameters to be calibrated, a sensitivity analysis was carried out. The parameters with a major effect on the behavior of the system were selected. The sensitivity of the system to the parameters was measured using the following equation:

$$S^{+} = \frac{(C^{+} - C)}{dP/P} \tag{3.18}$$

In this case, currencies are defined as biodiesel production and production capacity. The sensitivity analysis was carried out using the data reported in Table 3.8.

Biodiesel production and production capacity were chosen as criteria for model calibration. Figure 3.8 and Figure 3.9 show the values used. The mean squared error (MSE) was selected as a measure of model fit to time series. Simulations were run 6000 times per parameter in the sensitivity analysis and 200 times in the calibration of the model.

The MSE is defined as follows:

Table 3.6: Assumptions for bioenergy system parameters.

Parameter	Value	Unit	Description
Initial land[a]	2500000	ha	Total land of farmers
Initial biodiesel producers capacity	200	$Ml\,yr^{-1}$	Initial total capacity of biofuel producers
Initial rapeseed price	250	$€\,t^{-1}$	Initial rapeseed price
Initial wheat price	100	$€\,t^{-1}$	Initial wheat price
Initial biodiesel price	0.5	$€\,l^{-1}$	Initial biodiesel price
Time deployment new biofuel plant[b]	[2 – 5]	yr	It defines how long it takes to build a new biofuel plant
Subsidy decommissioning rapeseed[c]	100	$€\,t^{-1}$	Subsidy granted to the farmer for growing rapeseed
Subsidy decommissioning wheat[c]	43	$€\,t^{-1}$	Subsidy granted to the farmer for growing wheat
Net profit margin biofuel producers[d]	N(3,5)	%	Profit margin of biofuel producers
Net profit margin distributors[d]	N(3,5)	%	Profit margin of distributors
Total rapeseed demand	7	Mt	Maximum rapeseed demanded in the system
Ratio demand distribution capacity biofuelproducers	1.5	N.A	Ratio Capacity distribution to production capacity
Glycerol price[e]	500	$€\,t^{-1}$	Glycerol price
Rape meal price[f]	250	$€\,t^{-1}$	Rape meal price
Wheat price floor[g]	80	$€\,t^{-1}$	Minimum wheat price
Rapeseed price floor[g]	150	$€\,t^{-1}$	Minimum rapeseed price
Rapeseed price cap[g]	400	$€\,t^{-1}$	Maximum rapeseed price
Price difference rapeseed - wheat[g]	230	$€\,t^{-1}$	Price difference rapeseed and wheat

[a] Value estimated based on the agricultural land use for rapeseed in Germany [125].
[b] Uniform distribution
[c] Values calculated using the value of the standard agricultural premium ($301\,€\,ha^{-1}$) and the average yield value for rapeseed ($3\,t\,ha^{-1}$) and wheat($7\,t\,ha^{-1}$)
[d] Normal distribution N(X,Y); X = mean; Y = standard deviation
[e] Value estimated from Quispe et. al [126]
[f] Value estimated from UFOP [127]
[g] Values estimated from data reported in FAO [118]

Table 3.7: Assumptions for model specific parameters

Parameter	Value	Unit	Description
Number farmers[a]	90	#	Number of farmers
Number Biofuel producers[a]	30	#	Number of biofuel producers
Number distributors[a]	10	#	Number of distributors
Vision biofuel producers[a]	8	Patches	It is the distance that each biofuel producer can see 360 degrees around him
Vision distributors[a]	8	Patches	It is the distance that each biofuel producer can see 360 degrees around him
Base land conversion factor[b]	N(40,10)	%	It defines the initial fraction of arable land to be used to produce rapeseed
Rate land conversion factor[b]	N(20,10)	%	It defines the rate of expansion of the fraction of arable land to be used for rapeseed production
Biofuel producer exiting factor	2	N.A	Factor used to estimate the exiting criteria of biofuel producers. $ExitingCriteria = CAPEX \cdot Factor$. If the losses are greater than this criteria the biofuel producer will leave the system
Perception of the biodiesel market development	6	N.A	Factor used to estimate the number of new plants to be built. If conditions are favorable for investment, the biofuel producer will built a number of plants equal to this parameter
Recovery time biofuel producers	2	yr	It is the maximum time biofuel producers are allowed to make loses consecutively. If the cross this limit, they will leave the system

[a] Parameters used to create the network among farmers, biofuel producers, and distributors in the set-up of the model.
[b] Normal distribution N(X,Y); X = mean; Y = standard deviation

Table 3.8: Parameters used in the sensitivity analysis

Parameter	Reference value	Min value	Max value
Base land conversion factor	40	20	60
Rate land conversion factor	20	10	30
Perception of the biodiesel market development	2	1	3

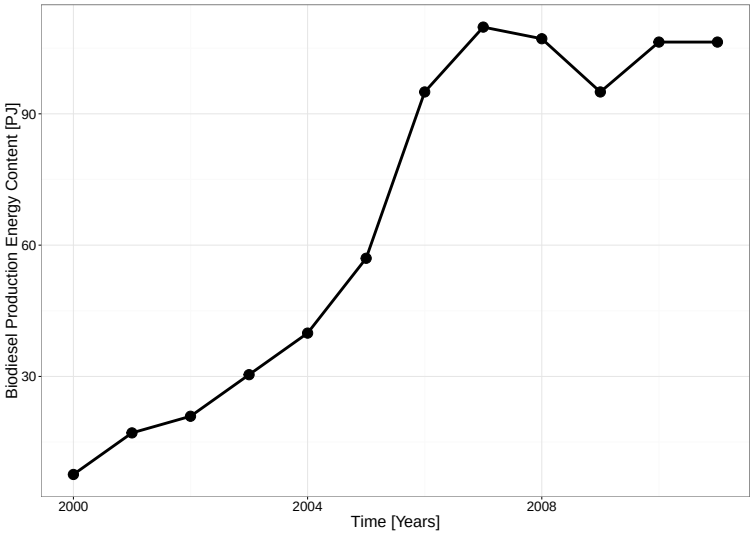

Figure 3.8: Biodiesel production: Historical data (adapted from Kaup & Selbmann [96]). An energy density of 33.4 MJ L^{-1} was used to calculate the energy content.

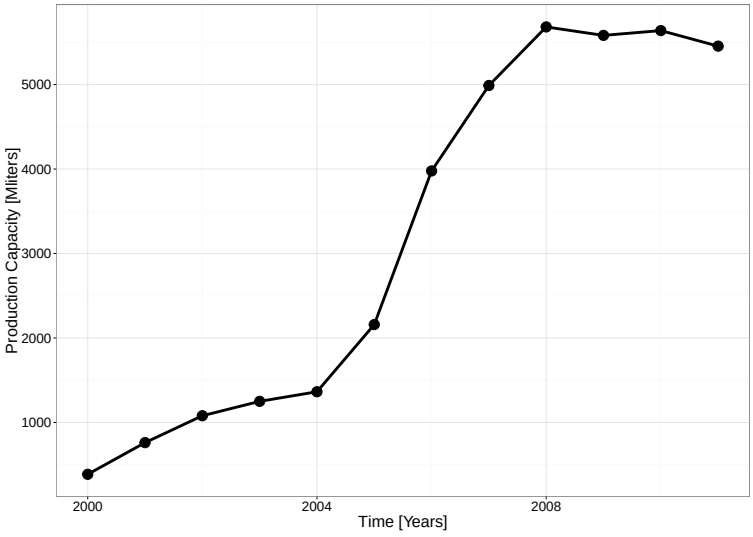

Figure 3.9: Biodiesel production capacity: Historical data (adapted from Kaup & Selbmann [96]).

$$MSE = \frac{\sum_{i=1}^{n} \hat{Y}_i - Y_i}{n} \tag{3.19}$$

An uncertainty analysis was carried out to determine the reliability of the model. The parameter "perception of the biodiesel market development", pmd, was assumed to exhibit a uniform discrete distribution in the range 2 to 10. A robustness analysis was also carried out to analyze *"whether a result depends on the essentials of the model or on the details of the simplifying assumptions"* [128]. Similar to the uncertainty analysis, it was assumed that the biofuel producer's perception of the biodiesel market development, pmd, exhibits a uniform discrete distribution in the range 1 to 6.

3.4. RESULTS

3.4.1. SENSITIVITY ANALYSIS

As discussed in Section 3.3, a sensitivity analysis was carried out to determine whether parameters with high uncertainty have a large influence on the behavior of the system. Figure 3.10 presents the sensitivity of biodiesel production and production capacity over time with respect to the parameters described in Table 3.8. Figure 3.10 shows that the biofuel producer's perception of the biodiesel market development, pmd, exerted a significant influence on the behavior of the system. Conversely, the initial fraction of land allocated by the farmer to produce energy crops, blc, and the rate of expansion of the fraction of arable land to be used for energy applications, rlc, had a minor impact on the system.

3.4.2. MODEL CALIBRATION AND VALIDATION

The model was calibrated by finding the value of the biofuel producer's perception of the biodiesel market development, pmd, which rendered the lowest MSE. Ranges for this parameter were determined based on the sensitivity analysis. Values for the parameter pmd varied between 1 and 20 units. The model was run 200 times for each permutation.

Figure 3.11 presents the mean squared error as a function of the parameter pmd. The calibration criterion used was biodiesel production reported in the period 2000-2011. The lowest value of MSE was found when the parameter pmd had a value of 6 units.

Figure 3.12 presents the mean squared error as a function of the parameter pmd. The calibration criterion used was production capacity reported in the period 2000-2011. The lowest value of MSE was found when the parameter had a value of 6.

3.4.3. BIODIESEL PRODUCTION AND PRODUCTION CAPACITY PATTERNS

Figure 3.13 shows biodiesel production as a function of time. The figure shows the median, the 50% and 90% envelope of the results obtained from the agent-based model developed in this study, using the value of 6 units for the parameter. Historical data reported by Kaup & Selbmann [96] is also presented in the graph. The model results exhibited a similar dynamic reported in the historical data: a step increase of biodiesel production in 2005 followed by two dips in production in 2009 and 2012. Model results, however, did not match the historical data. The highest deviations were reported in 2003 and 2012 with a percentage error of 66% and 59%, respectively. The lowest deviation was

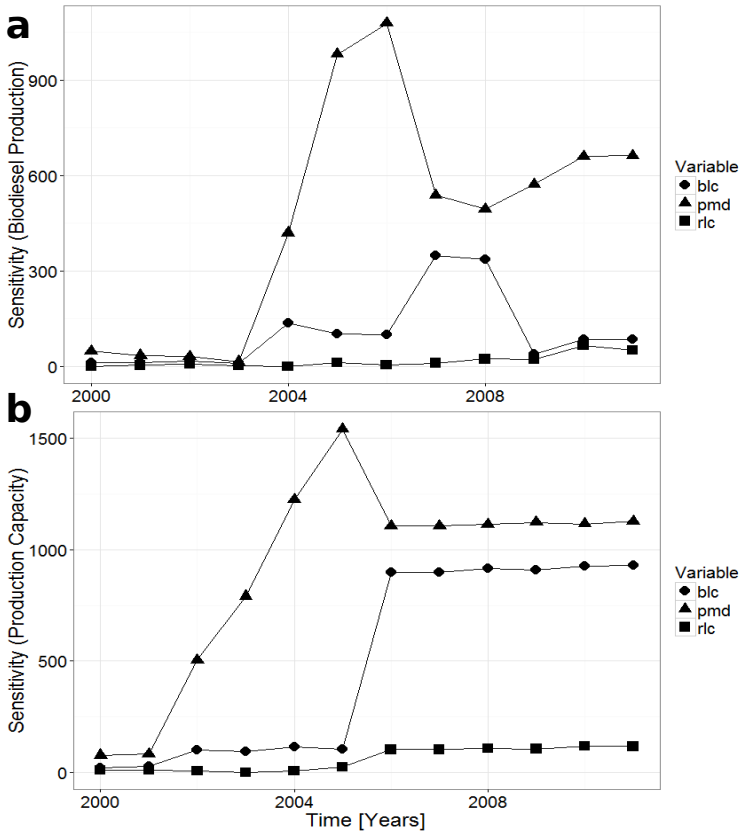

Figure 3.10: Partial derivative of biodiesel production (**a**) and production capacity (**b**) as a function of time.

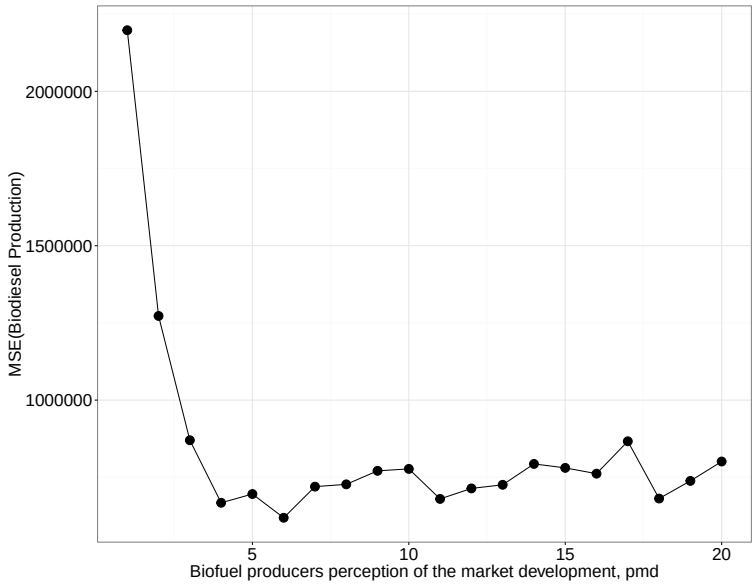

Figure 3.11: Mean squared error using the calibration criterion biodiesel production as a function of the biofuel producers' perception of the market development.

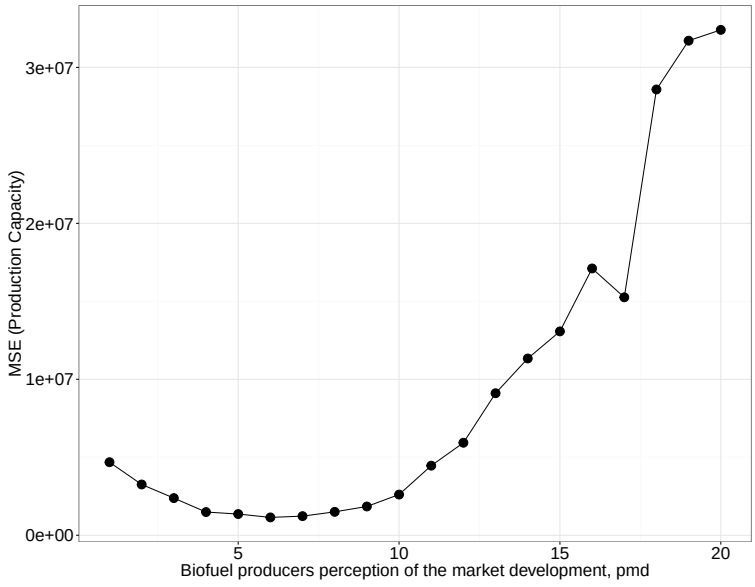

Figure 3.12: Mean squared error using the calibration criterion production capacity as a function of the biofuel producers' perception of the market development.

reported for the year 2006, with a percentage error of 12%. The percentage error was calculated by using the mean of the results obtained in the simulations.

In attempt to validate the model, historical data for biodiesel production in the period 2012 – 2014 were contrasted with the model results. Simulation results exhibited a plunge in biodiesel production in 2012, which was due to a low yield on rapeseed production in 2011 ($2.91\,\mathrm{t\,ha^{-1}}$) probably because of bad weather conditions. In reality, biodiesel production remained approximately constant because of the import of oilseeds. During the period 2006 – 2010 Germany imported an equivalent of 11% of the total oilseed imported by the EU, whereas in the period 2011-2012 Germany imports increased to 14% [129]. In 2013 and 2014, model results exhibited a different dynamic to that displayed in the historical data, which exhibited an increase in the biodiesel production. Simulation results did not exactly match historical data. The percentage of error was 38% and 47%, respectively.

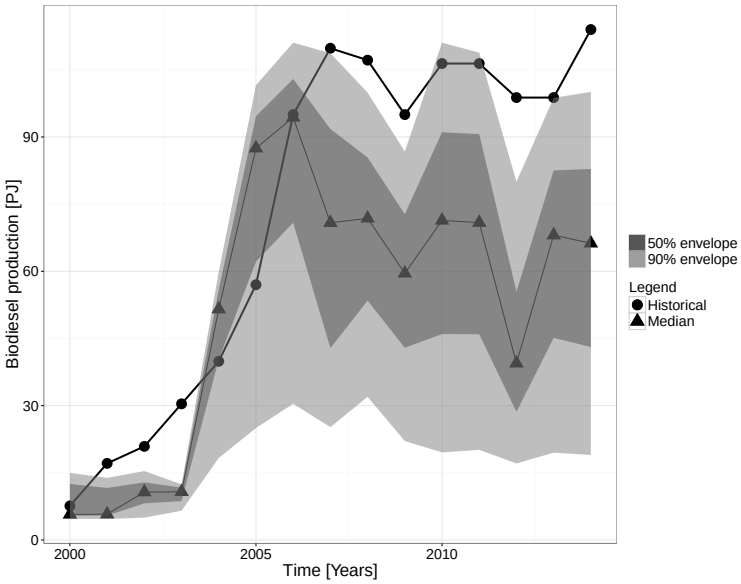

Figure 3.13: Biodiesel production as a function of time. Model results and historical developments.

Figure 3.14 shows production capacity as a function of time. Like Figure 3.13, this graph presents the median, the 50% and the 90% envelope of the results obtained from the simulation in addition to the historical data reported elsewhere [96]. Model results did not match the historical data. The highest deviation was reported for 2004, with a percentage error of 160%. The lowest deviation was reported for 2007, with a percentage error of 4%. However, the rate of expansion in production capacity predicted by the model exhibited a similar dynamic to that reported by the historical results. The main difference lay in the time that production capacity took off. The premature deployment of production capacity reported by the model is due to the assumption that the parameter is constant. In reality, investor's perception on expansion capacity gradually increased with the evolution of the institutional framework which benefited the

biodiesel industry before 2006.

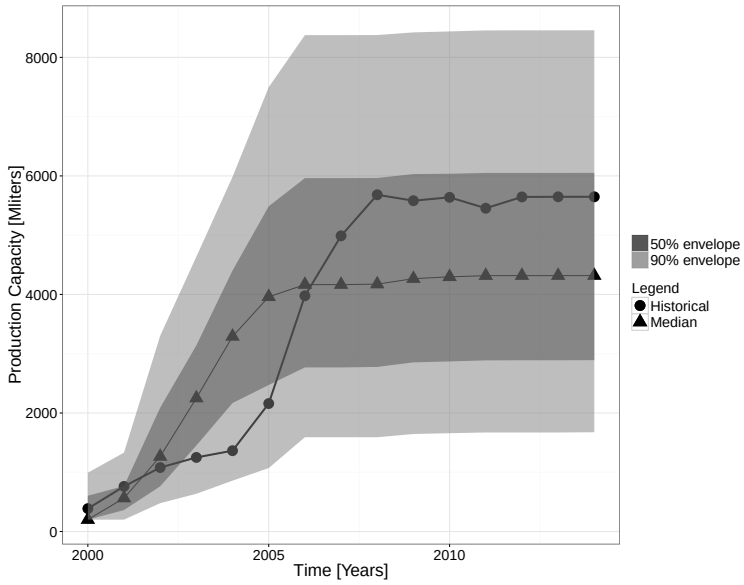

Figure 3.14: Production capacity as a function of time. Model results and historical development.

3.4.4. UNCERTAINTY ANALYSIS

An uncertainty analysis was carried out to evaluate how uncertainty in the calibration parameter affects the reliability of the model. Figure 3.15 shows how many simulation experiments out of 10 000 (y-axis) produced biodiesel production results within the ranges on the x-axis in different years. The uncertainty in the results for biodiesel production increased with time due to the dynamics in the system, primarily the investment (or divestment) in production capacity. After 2004, when a surge in biodiesel production and production capacity took place, the uncertainty in biodiesel production results increased considerably. Likewise, this uncertainty further increased in 2007 when many decisions on disinvestment were made.

3.4.5. ROBUSTNESS ANALYSIS

The sensitivity analysis showed that the biofuel producer's perception of the biodiesel market development, pmd, has a considerable influence in the system behavior. As this parameter was assumed to be equal to all biofuel producers, it is important to analyze whether the patterns generated depends on this simplifying assumption. To test model's ability to reproduce the biodiesel production and production capacity patterns when this assumption is relaxed a robust analysis was carried out. For a percentage p of the biofuel producers, the term:

$$pmd = a \tag{3.20}$$

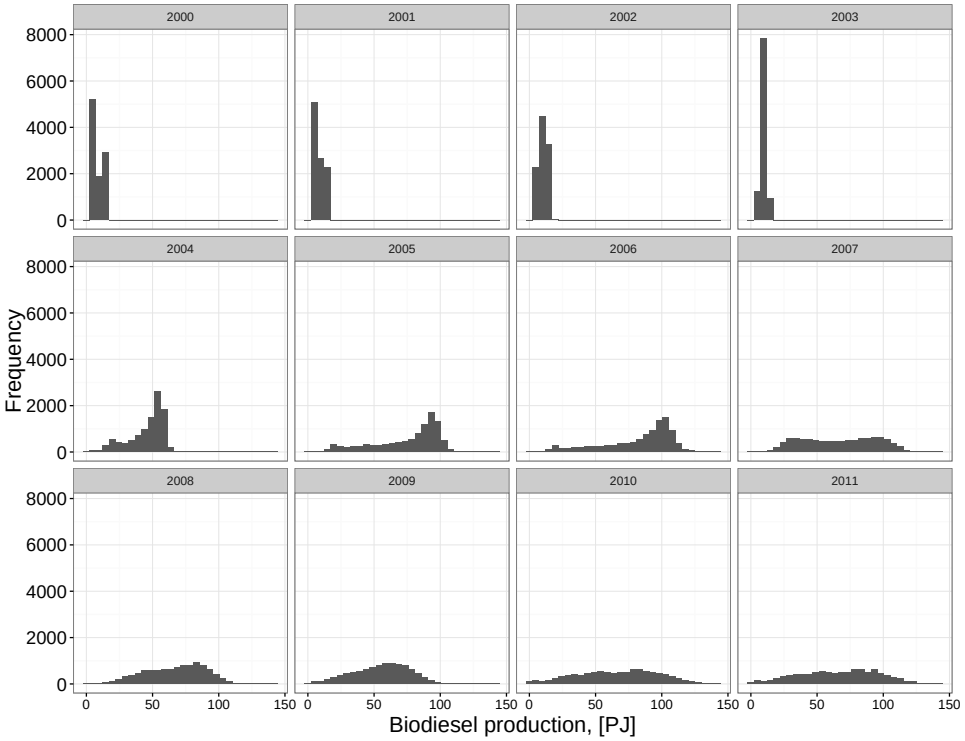

Figure 3.15: Uncertainty analysis for biodiesel production.

It was replaced by:

$$pmd = U(1, a) \tag{3.21}$$

Where a is a constant.

Figure 3.16 presents biodiesel and production capacity as a function of time for different percentage of biofuel producers with different perceptions (10 – 90%). The results showed that an increase in the percentage of biofuel producers with different perceptions had an insignificant effect on patterns in biodiesel production and slightly decreased the production capacity.

3.5. DISCUSSION

THE sensitivity analysis and model calibration suggest that the patterns in production capacity result from investors basing their decisions on optimistic perceptions of market developments. The influence of behavioral aspects, such as actors' perception, on biofuel supply chains behavior and how these aspects depend on the institutional framework has been already pointed out by van Vliet *et al.* [39].

In contrast, the historical patterns in biodiesel production can only be partly explained by this hypothesis. The difference in the description of system dynamics be-

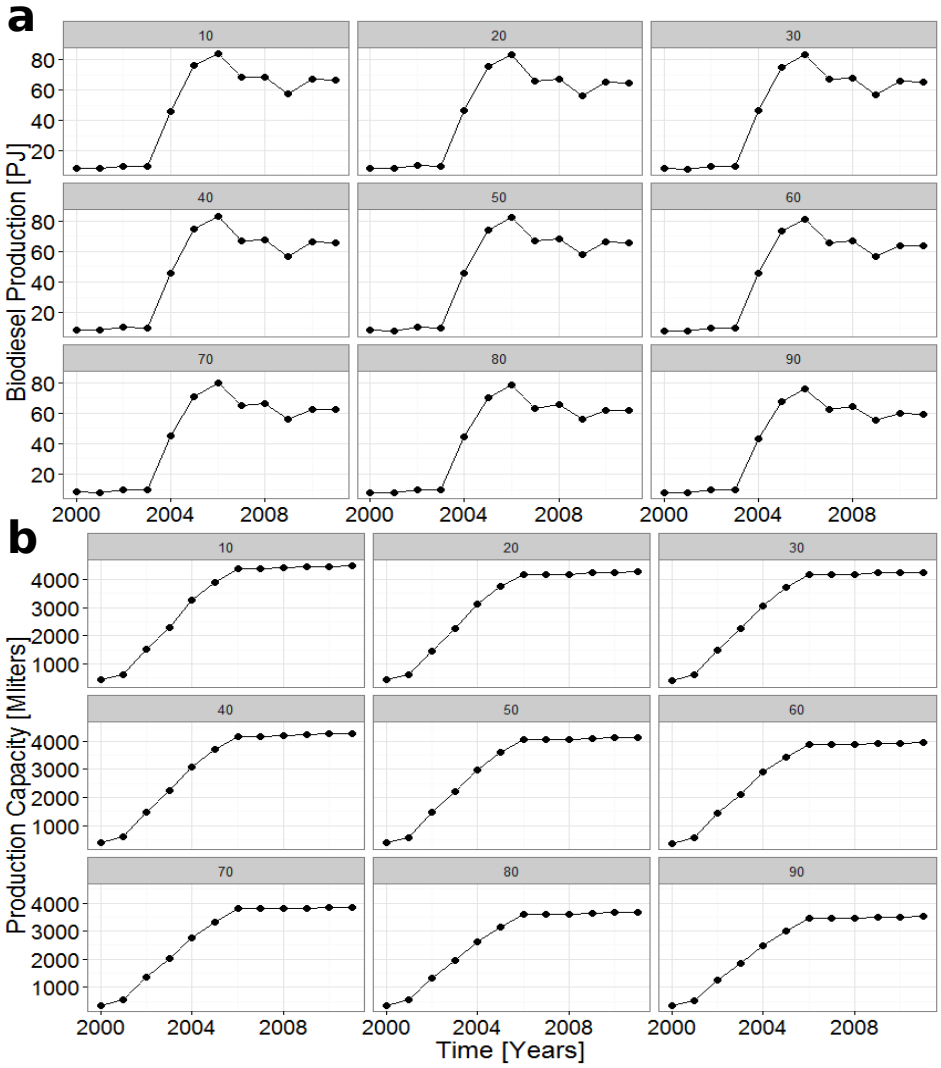

Figure 3.16: Biodiesel production (**a**) and production capacity (**b**) as a function of time at different percentage of biofuel producers with different perceptions of the market development.

tween the agent-based model and the historical developments as of 2006 may indicate that other important mechanisms impact system behavior. The authors suspect that those mechanisms are related to the opening of the German biodiesel market to the world. Since 2006 German imports of biodiesel [112] and rapeseed oil have increased [129]. This interaction with the world market was neglected as the biodiesel and rapeseed market in Germany was assumed to be a closed system.

Discrepancies between model results and historical data regarding the rate of expansion of production capacity are due to assumptions about the biofuel producer. In the model, biodiesel producers have a perception of the market that suddenly becomes optimistic with the introduction of a favorable institutional framework. In reality, actors' perception on the system is gradually influenced by institutions (i.e. property rights, rule of law, financial system, incentives, etc.) as it has be pointed out by North [73].

Discrepancies in the rate of expansion of biodiesel production are due to underlying assumptions. It was assumed that during the agricultural reform period (1992-2002), rapeseed (for non-food applications) is only grown in the set-aside land. In reality, rapeseed was also grown in arable land and biofuel producers could either source it locally or import oilseeds [112].

Parameters such as the initial fraction of arable land to be used to produce rapeseed allocated by the farmer, blc, and its rate of expansion, rlc, have a negligible effect on the biofuel supply chain because of the stabilizing feedback mechanisms incorporated in the model. That is, farmers decide whether to expand rapeseed production based on what they sold in the last season. If farmers manage to sell their entire crop, they will expand their cultivation. Otherwise, they will grow an amount equivalent to what they sold in the previous year.

On the other hand, the uncertainty analysis further indicates that the model could be used to simulate differences among scenarios. One should be cautious with any absolute predictions from the model as uncertainty increases with the course of the simulation. The robustness analysis results indicate that the assumption of a shared perception on market development among biofuel producers (i.e. all biofuel producers have the same value for the parameter pmd) is robust enough. Differences in perception had a slight influence on patterns in biodiesel production and production capacity. This finding is in line with the process of stabilization and convergence of actors' expectations claimed by strategic niche management authors [95].

From a theoretical point of view, framing a biofuel supply chain as a complex adaptive system enables the incorporation of concepts such as emergence, adaptation, learning, and bounded rationality, which are seldom thought of in an optimization. In this agent-based model we translate these concepts as follows: patterns in biodiesel production and production capacity emerge as a result of the interaction between farmers, biofuel producers, and distributors. Those actors are heterogeneous and operate according to their own preferences. As it is assumed that these agents have bounded rationality (i.e. limited processing information capacity and limited information), they forecast markets developments. Adaptation mechanisms are incorporated in the forecasting process. As the agents know more about the markets, forecasts are improved. This is in sharp contrast with the optimization approach where such elements are neglected.

The conceptual framework proposed offers an alternative for thinking about bio-

fuel supply chains and describing agent-based models. Previous thinking about the economics of biofuel supply chains has been reductionist. The effects of technologies [79, 80], policy [27] and management [28, 87] on biofuel supply chain behavior have been independently analyzed. Therefore, the interaction between these elements and its effect on the system is not well understood yet. The consequences of these interactions can be understood by simulation.

Moreover, the conceptual framework enables the incorporation of social structures into an agent-based model right from the conceptualization phase. This is in sharp contrast with the standard agent-based models for biofuel supply chains, where social structures are not considered or are considered as part of the agents [38, 40, 42]. The use of agents with internal social structures is far from reality, as these structures are observed as independent concepts within social systems. In fact, social structures emerge from individual behavior and social interaction [61]. The introduction of social structures as an independent concept should be a way to cope, right from the start, with the complexity of socio-technical phenomena.

Although a traditional approach might provide results that adequately fit the macroscopic patterns, it cannot provide further insights about what mechanisms and processes are relevant to explain them. The formalization of the proposed conceptual framework into an agent-based model offers a means of explanation. The simulation model can be used to test hypothesis that aim to explain the phenomenon of interest. In this study, we tested the hypothesis that patterns in biodiesel production and production capacity results from investors' perception of market development. However, the explanatory force of the model is limited by the uncertainty in the data. Lack of qualitatively and quantitatively data about investors' perceptions is one of the main limitations of the approach. The proposed method could be used to systematically explore different mechanisms that might lead the system to the direction pointed by studies based on optimization. Specifically, the methodology proposed in this work could be used to analyze different deployment strategies for both existing and new bioenergy systems, such as the production of renewable jet fuel from biomass.

This approach, however, does have several limitations. Firstly, it neglects spatial considerations and network structures. Understanding processes of spatial diffusion lies outside the scope of this paper. Network structures, however, can have an important effect on the performance of the system. As was pointed out by Strogatz [130] *"structure always affects function"*. Furthermore, although some non-economic attributes (e.g. bounded rationality and expectations) were incorporated into the agents' decision making, there is room for improvement. Farmers' decision making should include non-economic attributes such as willingness to grow energy crops, risk preferences, and network effects that have proven to be a barrier to the adoption of energy crops [38]. Despite these limitations, the case study developed in this research gives more evidence on the importance of the incorporation of social elements (actors, and institutions) in the analysis of (bio) energy systems. The replication of past behavior of the system by identifying the central causal mechanisms offers important practical applications such as the assessment of past and future policy interventions. The ABM developed in this study might be used to extend the analysis done by Kaup & Selbmann [96] by considering path dependencies and the interaction among agricultural and biofuel policies.

3.6. CONCLUSIONS

IN this study, we aimed to analyze the emergence of patterns in biodiesel production and production capacity in Germany as a result of the interaction of three elements: physical system, network of actors, and institutions. The production of biodiesel from rapeseed in Germany has been conceptualized based on elements of complex adaptive systems, socio-technical systems, and (neo) institutional economics. These concepts were formalized using the agent-based modeling approach (ABM).

For the specific case study, considering the sensitivity analysis and model calibration results, we argue that the dynamics in production capacity could be explained by the hypothesis that these patterns emerge from investors basing their decisions on optimistic perceptions of the market development. However, patterns in biodiesel production cannot be completely explained with this hypothesis due to increasing imports of rapeseed and biodiesel from 2006 onwards, which were not included in the model. Thus, an analysis of the interaction of global rapeseed and vegetable oil markets with the German biodiesel supply chain and its effect on biodiesel production is recommended. It is also recommended to improve farmers' decision making by adding non-economic attributes such as risk preferences and network effects into the model. Accounting for these concepts in decision making is one of the advantages that set apart agent-based modelling from traditional economic approaches such as computational general equilibrium models.

In light of the robustness analysis results, we conclude that the assumption that all biofuel producers have the same perception of market developments is robust. This finding is in line with the process of stabilization and convergence of actors' expectations presented in the strategic niche management framework.

The proposed conceptual framework offers an alternative analytical tool to study biofuels supply chains in general. The framework recognizes that a biofuel supply chain is more than a technological construction or organizational construction. In fact, it proposes that a biofuel supply chain is the result of the interaction between these two constructs. The conceptual framework enabled the incorporation of social structures into an agent-based model from the conceptualization phase.

One concrete advantage of the proposed method is exploited when the conceptual framework is formalized into an agent-based model. The computational model, besides facilitating the systematic exploration of the consequences of the interaction among physical components, actors, and institutions on the German biodiesel supply chain behavior, it also offered a test bed for hypothesis of the system behavior. The approach proposed in this study could be used as a means to explore different mechanisms that might lead to the equilibrium predicted by the studies based on optimization. Specifically, this approach could be used to provide insights on the effect of different future deployment strategies on bioenergy systems development.

This study simply lays out a first step in the institutional analysis of biofuel supply chains. A further step would be the use of the model to construct alternative scenarios, e.g. to assess the impact of certain policy interventions. This will be done in future studies. Due to high uncertainty in the model results, it is recommended to make relative predictions. Finally, as this study carried out a high-level system analysis it would be interesting to focus on particular elements of the system. For instance, the influence

of policies on the organizational structures of farmers and biofuel producers might be worthwhile to investigate.

3.7. NOMENCLATURE

3.7.1. MATHEMATICAL SYMBOLS

a: parameter used in Equation (3.11)
blc: base land conversion factor. It defines the initial fraction of arable land to be used to produce rapeseed allocated by the farmer.
C^+: value of the currency evaluated in the point $P^+ = P + dP$
C: value of the currency evaluated in the point P.
C^e_{t-1}: estimate for the variable C in the time $t-1$
C_{t-1}: actual value of the variable C from the time $t-1$
C^e_t: Updated estimate of the variable C for the time t
c_{b_j}: fixed cost of the refinery operated by the biofuel producer j, [€l^{-1}]
Cap_j: capacity of the refinery owned by the biofuel producer j, [Ml yr^{-1}]
L: distance calculated in the simulation between either a farm and a biodiesel plant or between a biodiesel plant and a distributor center. [km]
lc: conversion factor to account for the different scale between the spatial dimensions used in the simulation and the real ones in Germany.
MC_{b_j}: marginal cost of producing biodiesel in the refinery owned by the biofuel producer j, €l^{-1}
MSE: mean squared error.
n: number of predictions.
P_b: wholesale biodiesel prices, [€l^{-1}]
P_d: diesel price, [€l^{-1}]
P_g: glycerol price, [€t^{-1}]
P_{rm}: rape meal price, [€t^{-1}]
P_r: rapeseed price, [€t^{-1}]
$P^{bid}_{r_j}$: rapeseed price bid in the market for the biofuel producer j, [€t^{-1}]
$P^{bid}_{bp_k}$: biodiesel producer price bid into the market by the distributor k, [€l^{-1}]
$P^{exp}_{b_k}$: expected biodiesel price of the distributor k, [€l^{-1}]
$P^{exp}_{bp_j}$: expected biodiesel producer price of the biofuel producer j, [€l^{-1}]
$P^{exp}_{r_j}$: expected rapeseed price, [€t^{-1}]
PM_j: profit margin for the biofuel producer j.
PM_k: profit margin for the distributor k.
pmd: perception of the biodiesel market development. This parameter is used to simulate the perceptions of investors in the German biodiesel market. This parameter is translated into the number of new plants to be built and it is a function of the biodiesel tax and quota.
q_b: biodiesel quota, [Ml yr^{-1}]
q_{b_j}: volume of biodiesel to be produced, [l]
q_r: Mass of rapeseed to be processed, [t]
rlc: rate land conversion factor. It defines the rate of expansion of the fraction of arable

land to be used for rapeseed production allocated by the farmer.
S_+: partial derivative of the currency C with respect to the parameter P.
TC_{b_j}: total production cost of biodiesel, [€l^{-1}]
tc: unit transportation cost of the good b or r, [€l^{-1}, €t^{-1}]
t_b: biodiesel tax, [€l^{-1}]
tc_p: transportation cost of the product b or r, [€l^{-1}km^{-1}, €t^{-1}km^{-1}]
Y_{b-g_j}: yield glycerol of the biofuel producer j, $[\mathrm{kg}_{\mathrm{glycerol}}\,\mathrm{kg}^{-1}_{\mathrm{biodiesel}}]$
Y_{o-b_j}: yield of biodiesel from oil rapeseed of the biofuel producer j, $[\mathrm{kg}_{\mathrm{biodiesel}}\,\mathrm{kg}^{-1}_{\mathrm{oilrapeseed}}]$
Y_{r-o_j}: yield of oil from rapeseed of the biofuel producer j, $[\mathrm{kg}_{\mathrm{oilrapeseed}}\,\mathrm{kg}^{-1}_{\mathrm{rapeseed}}]$
Y_{r-rm_j}: yield of rapeseed meal from rapeseed of the biofuel producer j, $[\mathrm{kg}_{\mathrm{rapeseedmeal}}\,\mathrm{kg}^{-1}_{\mathrm{rapeseed}}]$
$\hat{Y}_i$: vector of n predictions.
Y_i: vector of observed values

3.7.2. GREEK SYMBOLS

ρ_b: biodiesel density, [kgl^{-1}]
λ: milles per galon diesel equivalent

3.7.3. ABBREVIATIONS

b: biodiesel
g: glycerol
$i \in I$: set of all farmers
$j \in J$: set of all biofuelproducers
$k \in K$: set of all distributors
r: rapeseed
rm: rapeseed meal
ro: rapeseed oil

4

INSTITUTIONAL ANALYSIS OF THE GERMAN BIODIESEL SUPPLY CHAIN

In all fiction, when a man is faced with alternatives
he chooses one at the expense of others.
In the almost unfathomable Ts'ui Pen,
he chooses—simultaneously—all of them.
He thus creates various futures, various times which start others that
will in their turn branch out and bifurcate in other times ...
this web of time—the strands of which approach one another, bifurcate,
intersect or ignore each other through the centuries—embraces every
possibility. We do not exist in most of them. In some you exist and not I,
while in others I do, and you do not, and yet in others both of us exist.

Jorge Luis Borges, *The garden of forking paths*

This chapter has been published as Moncada, J.A., *et al.*, Exploring path dependence, policy interactions, and actor behavior in the German biodiesel supply chain. Applied Energy, 2017. 195: p. 370-381.

Biofuel production is not cost competitive and thus requires governmental intervention. The effect of the institutional framework on the development of the biofuel sector is not yet well understood. This chapter aims to analyze how biofuel production and production capacity could have evolved in Germany in the period 1992 - 2014. *The effects of an agricultural policy intervention (liberalization of the agricultural market) and a bioenergy policy intervention (a tax on biodiesel after an initial exemption) are explored. Elements of the Modeling Agent systems based on Institutional Analysis (MAIA) framework, complex adaptive systems (CAS) theory, and Neo Institutional Economics (NIE) theory were used to conceptualize and formalize the system in an agent-based model. It was found that an early liberalization of the agricultural market led to an under-production of biodiesel; a late liberalization led to the collapse of biodiesel production. An early introduction of the biodiesel tax led to stagnation in biodiesel production and production capacity; a late introduction led to an increase in sunk costs provided that the biofuel quota is binding. Also, a lack of agents' adaptation mechanism to forecast prices led to a decrease in patterns of biodiesel production when an external shock was introduced in the system. In sum, we argue that system behavior is influenced by individual behavior which is shaped by institutions.*

4.1. INTRODUCTION

CONCERN has grown in the last decades over the issue of climate change. Strategies to tackle this problem include the production of energy from solar, wind, biomass, and other renewable sources. In Europe, the production of liquid fuels from biomass has gained considerable momentum due to its potential to reduce greenhouse gas emissions, to enhance energy security through the substitution of fossil fuels, and to contribute to rural development by increasing employment opportunities[1] and diversifying the activities of farmers [97, 132].

Despite the benefits of biofuels, biofuel production is not cost-competitive and thus requires governmental intervention. Policy instruments such as blending mandates, tax credits or tax exemptions, subsidies, and import tariffs are used to stimulate biofuel production and consumption in the world [18]. The literature has focused on reducing the price gap between biofuels and fossil fuels by optimizing the whole supply chain [21, 133–135], by improving the logistics [136, 137], and developing more efficient technologies [138–140]. There is clear evidence that biofuel supply chains cannot be created and developed in absence of governmental support[2] [18, 142], and yet the scientific literature has focused primarily on technological developments [139, 140, 143, 144] and their optimization [19, 20, 82].

The impact of policies on biofuels production is mostly analyzed by using an equilibrium framework [133, 145–147]. This approach has provided many insights by identifying promising configurations for feedstock, technology, and production capacity required to meet some policy goals. However, there is still a lack of understanding as to: what alternative stories (scenarios) could have unfolded as a result of different policy interventions; what the effects of policy interaction are on biofuel supply chain development and actors' behavior; and what strategies might steer the development of biofuel supply chains in the direction pointed to by the optimization studies.

4.1.1. LITERATURE REVIEW

Support schemes to promote the production and consumption of renewable energy are a key instrument in the decarbonization of the energy mix. The most common support schemes include the competitive auctions, the feed-in tariff scheme, and tradable green certificates [148, 149]. Socio-economic policies such as job creation and energy access have also influenced the deployment of renewable energy [150]. In the specific case of biofuels, policies such as: the Renewable Fuel Standard (RFS2) in the USA, the Common Agricultural Policy (CAP) and the Renewable Energy Directive (RED) in the EU have contributed to its deployment [18].

Traditionally, the analysis of the effect of policies on biofuel supply chains has been done by using an equilibrium approach. Luo and Miller [151] used game theory to model biomass and ethanol production decisions and to calculate the incentives required to drive farmers and ethanol producers to participate in cellulosic biofuel industry. Newes *et al.* [152] used the Biomass Scenario Model to understand the role of incentives on the

[1] Borenstein claims that these arguments, also used to promote renewable electricity generation, are difficult to support [131].

[2] As it was pointed out by van den Wall *et al.* bioethanol production in Brazil is a unique biofuel supply chain, as it no longer receives governmental support [141].

evolution of the cellulosic ethanol sector. The authors found that multiple points of intervention could accelerate the expansion of that biofuel industry. Rahdar *et al.* [153] developed a linear programming model to study the competition between biopower generation and biofuel production under the Renewable Portfolio Standards and renewable Fuel Standard in the U.S. The authors found that cellulosic biofuel production will dominate the competition for biomass against biopower generation. Christensen and Hobbs [27] developed a mathematical model of the U.S. biofuel market. The authors argued that compliance with California biofuel policy requires rapid deployment of clean diesel fuels.

The above-mentioned studies do not completely capture the complex nature of biofuel supply chains (BSCs). BSCs are complex adaptive systems and thus they are highly non-linear, exhibit multi-scale behavior and path-dependence, evolve and self-organize making it difficult for an equation-based model to capture their characteristics [154]. By using models that lack this complexity, such as optimization models, is possible to make policy recommendations and to design optimal supply chains. But that optimality only applies in a limited context. As it was pointed out by Simon in his famous Nobel prize lecture: *"decision makers can satisfice either by finding optimum solutions for a simplified world, or by finding satisfactory solutions for a more realistic world"* [155].

Path dependence is one of the interesting properties of complex adaptive systems [104]. The concept of path dependence is defined as a self-reinforcing mechanism [156] and as an outcome (lock-in). Verne and Durand define path dependence *"as a property of a stochastic process which obtains under two conditions (contingency and self-reinforcement) and causes lock-in in the absence of exogenous shock"* [157]. As a theoretical framework, path dependence has been used to explain institutional persistence [73], governance [158], and technology outcomes [159, 160]. However, as these are historical case studies it is difficult to provide strong evidence of history dependence [161].

A promising alternative to address these issues is Agent-Based Modeling (ABM). Concepts such as: emergence, adaptation, learning, and feedback mechanisms can be incorporated into ABM [37, 48]. As a simulation method, ABM can be employed to *"generate multiple historical trajectories emanating from the same set of initial conditions, thus enabling them to generalize about the mechanisms and processes that produce such histories"* [162]. That is, ABM can be utilized to analyze path dependence.

ABM has been used to address the effects of policies on both agricultural and bioenergy sectors. Brady *et al.* [163] extended the agent-based agricultural policy simulator (AgriPoliS) to understand the impact of agricultural policies on land use, and biodiversity. Brown *et al.* [164] assessed the bioenergy crop uptake as a function of farmer types and policy initiatives.

Some studies specifically analyze the impact of policies on biofuel supply chain performance by using the ABM paradigm. Agusdinata *et al.* [165] developed an agent-based model to understand the dynamics of biofuels supply chain networks. It was found that the network behavior is very sensitive to the rate of information feedback. Shastri *et al.* [42] analyzed the impact of policies on the evolution of a biofuel supply chain using an agent-based modeling approach. The authors argued that regulatory mechanism such as Biomass Crop Assistance Program led to greater productivity. Other studies have used the agent-based model approach to analyze the path dependence of network industries

under different policy regimes [166].

The contribution of this work is to extend the analysis of the effect of policies on the development of biofuel supply chains to account for the path dependence, policy interaction and effects on actor behavior. To achieve this goal, the German biodiesel supply chain was conceptualized and formalized by using an agent-based modeling approach. Biodiesel production in Germany was selected as a study case since it has been heavily influenced by governmental intervention [96, 97] as shown in Figure 4.1.

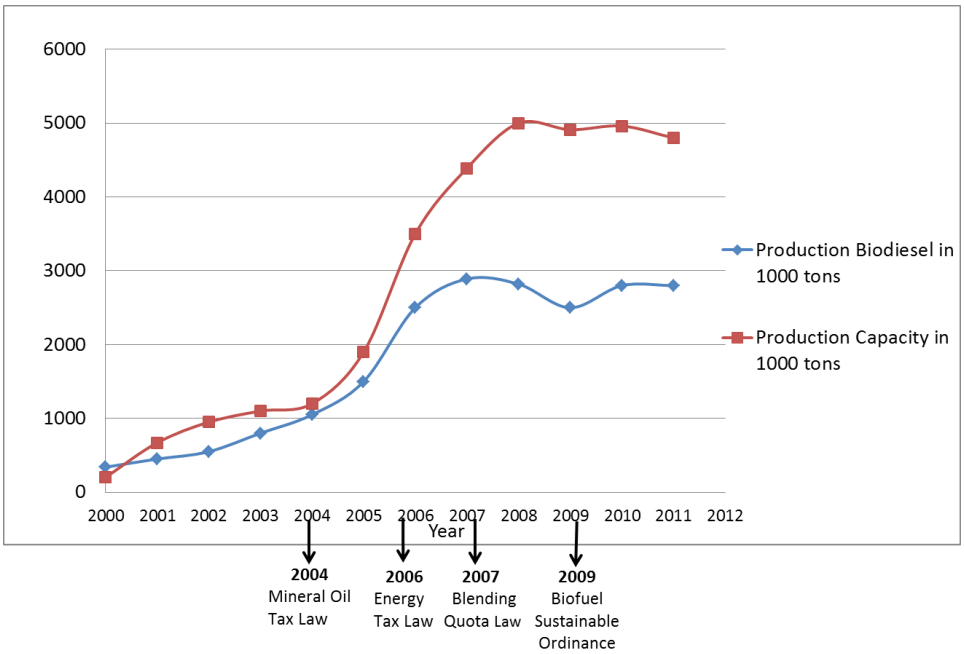

Figure 4.1: Effect of different policy interventions on biodiesel capacity and production [96].

The aim of the model is to shed light on how the German biodiesel industry could have evolved under different institutional frameworks and to assess the impact of biofuel policy instruments on biodiesel production and production capacity. Specifically, the research question is: *what patterns in biodiesel production and production capacity are generated as a result of applying different policy interventions in Germany in the period* 1992 - 2014*?*

The remainder of the chapter is organized as follows. Section 4.2 describes the development of the agent-based model and the data used in the experiments. Section 4.3 describes the results obtained which are discussed in Section 4.4. Conclusions are presented in Section 4.5.

4.2. THEORY AND METHODS

4.2.1. STRUCTURE OF THE AGENT-BASED MODEL

The construction of the agent based model starts with the formulation of the problem[3]. The problem is formulated using the generative science approach[4] [98], which identifies and describes the problem based on a macroscopic regularity or pattern[5] in the real world. The aim of the agent-based model is to understand how biofuel production and production capacity could have evolved as a result of different agricultural and/or bioenergy policy interventions. The impact of these policies on the different actors involved in the supply chain for biodiesel are to be modeled, replicating not only the currently observed pattern, but also exploring what conditions might lead to different outcomes.

At the core of the modeling framework is the concept of socio-technical systems. Usually, to describe a socio-technical system three elements are required: physical system, network of actors, and institutions [72]. The physical system entails resources (natural resources, information, and technical elements) present in the system. Actors are the agents that perform actions in the system. Institutions are defined as *"the rules of the game in society"* and their *"major role in a society is to reduce uncertainty by establishing a stable (but not necessarily efficient) structure to human interaction"* [73]. Neo institutional Economics (NIE) theory was used to describe the interaction between actors and institutions.

The physical system consists of feedstocks (rapeseed and wheat) and products (diesel and biodiesel); information regarding to prices for rapeseed, wheat, biodiesel, and diesel; and objects such as farms, refineries and distribution centers. The institutions are represented by the different agricultural and biofuel policies that took place in the period 1991-2014. The emergent behavior of the system is the result of the interaction among different actors (farmers, oil mill companies, biodiesel producers, distributors and gas stations), institutions, and the physical system.

Figure 4.2 presents a biofuel supply chain conceptual scheme. Agents interact with the objects (technologies) through ownerships (grey line). They interact with other agents by means of physical flows of rapeseed, oil, and biodiesel (solid grey arrow) and through the flow of money (dotted gray arrow). The decision making of different agents is based on the information (prices) provided by different markets (dotted black arrow). The environment is composed of the government. The government can influence the price of the different products and the behavior of the agents through incentives and/or mandates (solid black arrow). To simplify the analysis only three types of agents are included in the model: Farmers, biodiesel producers, and distributors. The environment of the system is composed of the German government which through policies, incentives, and regulations affects some or all of the agents mentioned above.

Figure 4.3 outlines the model narrative used in this study. The first year can be con-

[3] The model development is described in detail in Moncada *et al.* [167]

[4] *"To the generativist - concerned with formation dynamics - it does not suffice to establish that, if deposited in some macroconfiguration, the system will stay there. Rather, the generativist wants an account of the configuration's attainment by a decentralized system of heterogeneous autonomous agents." [98]*

[5] *"Patterns are defining characteristics of a system and often, therefore, indicators of essential underlying processes and structures. Patterns contain information on the internal organization of a system, but in a "coded" form." [168]*

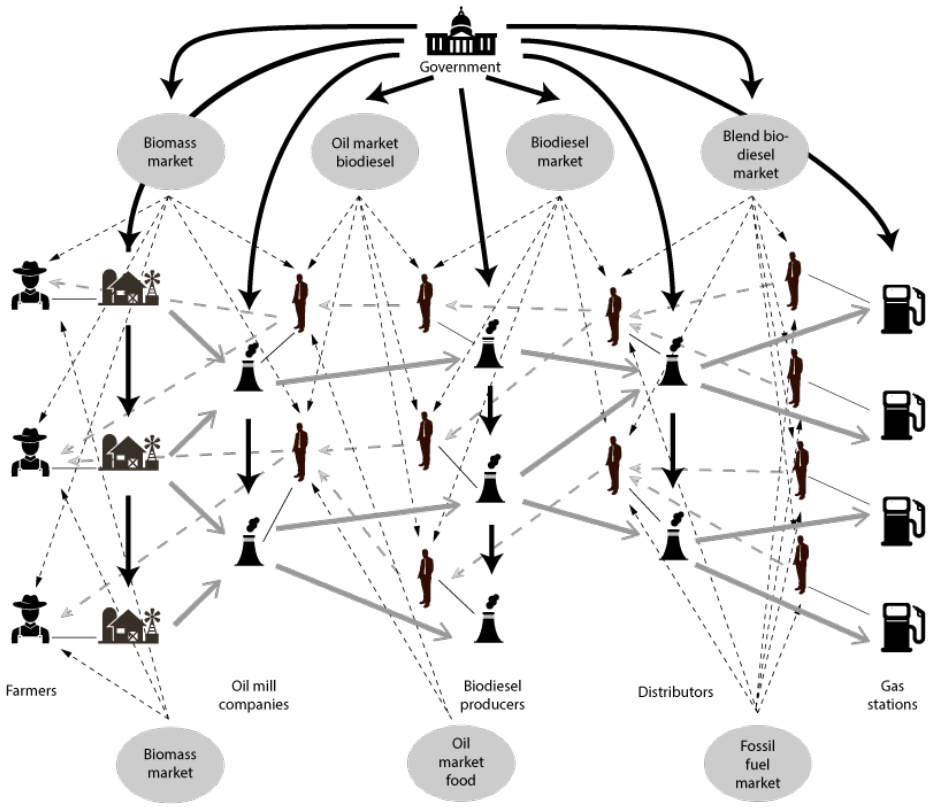

Figure 4.2: Biofuel supply chain conceptual scheme

sidered as a "warm up" period for the simulation. In this year farmers make decisions about land use under endogenous expectations. Biofuel producers and distributors determine theirs bids for rapeseed, and biodiesel, respectively, based on their forecasting. Also, rapeseed is sourced by biofuel producers. In the second year, biodiesel is produced and traded in the biodiesel market between biofuel producers and distributors. Investment decisions in production capacity are made by biofuel producers based on market developments. The activities described in the first year for the rapeseed market are also carried out in parallel during the second year. The cycle is repeated until the simulation reaches the final year.

The agent-based model incorporates typical characteristics of complex adaptive systems such as: adaptation, feedback effects, and heterogeneity. Farmers, biofuel producers, and distributors constantly adapt their forecast about prices for rapeseed, biodiesel producer price, and biodiesel price (consumer prices), respectively, based on feedback received from markets. Agents that share the same properties are assigned different values in those parameters. For instance, biofuel producers are assigned different values of production cost.

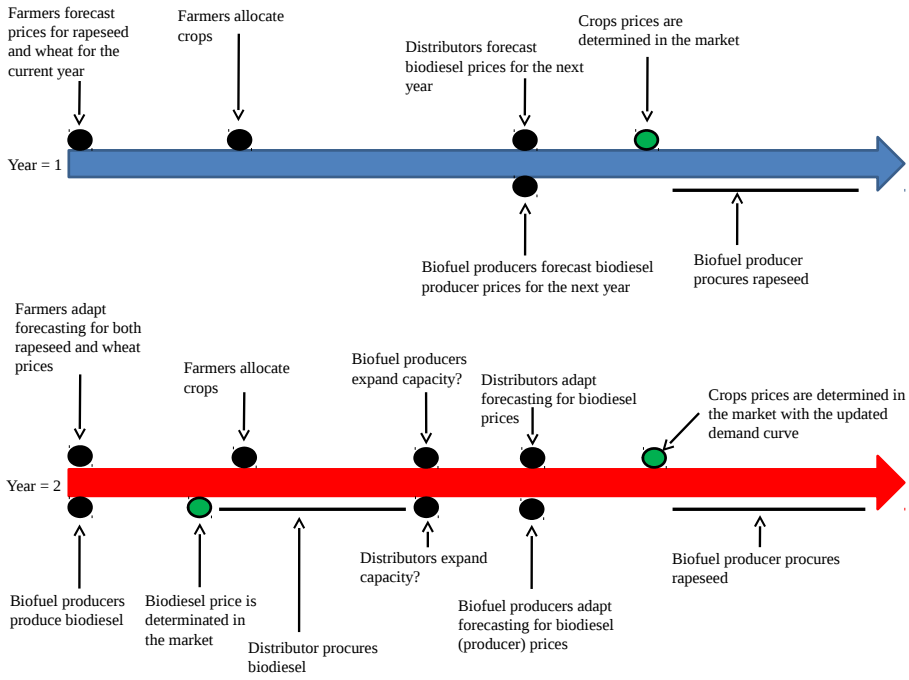

Figure 4.3: Model narrative

The concept of institution was formalized by using the MAIA framework [62] and the ADICO syntax [60]. ADICO refers to the five elements that an institutional statement can comprise: Attributes (designated roles), Deontic (prohibition, obligation, permission), aIm, Condition (for the institution to hold), and "Or else". Table 4.1 presents the conceptualization of institutions by applying the ADICO syntax. It was assumed that institutions are exogenous. Both policies, the agricultural reform and the liberalization of the agricultural market, influence farmers' decisions on crop allocation. The biofuel quota act influences biofuel producers' decision making on rapeseed procurement. The energy tax act affects the profitability of the biofuel producer.

Table 4.1: Institutional table for the biodiesel energy system (adapted from Moncada *et al* [167])

Institution						
Name	Attribute	Deontic type	Aim	Condition	Or else	Type
Agricultural reform	Farmer	must	sells crops to the energy market	If crops were grown in the earmarked land	Fine selling	Rule [a]
Liberalization of the EU agricultural market	Farmer		sells crops to the energy market	If prices in the energy market are equal or high to those prices in the food market regardless of the land type		Shared strategy[b]
Energy Tax act	Biofuel producer	must	Pays tax	If energy tax is binding	Fine producing	Rule
Biofuel quota act	Biofuel producer	must	Produce the amount of biodiesel assigned to meet the demand	If biofuel quota is binding	Fine producing	Rule
	Biofuel distributor	must	Distributes the amount of biodiesel assigned to meet the demand	If biofuel quota is binding	Fine distributing	Rule

[a] Rule: it includes all the elements of the ADICO syntax. That is, “attribute”, “deontic type”, “aim”, “condition”, and “or else”
[b] Shared strategy: it includes all the elements of the ADICO syntax but “deontic type”, and “or else”

The agricultural reform refers to the common agricultural policy (CAP) enacted in 1992. This policy decommissioned a percentage (5–15%) of agricultural land to be earmarked, or set aside, for alternative uses. Farmers were allowed to cultivate non-food crops on those set-aside lands. However, it was forbidden to sell set-aside rapeseed in the food market. A financial penalty was imposed on farmers who disobeyed this rule. The liberalization of the EU agricultural market prompted (or initiated) the fundamental reform of the CAP in 2003. Production- and volume-focused policies were shifted to area related payments to stimulate a further liberalization of the EU agricultural market.

The energy tax act specifies the energy tax law enacted in 2006. This biofuel policy defined an annual increase of the tax rate on biodiesel. The biofuel quota act refers to the biofuel quota law introduced in 2007. The aim of this policy was to stimulate the biodiesel industry by pressuring biofuel producers and distributors, to meet a biodiesel quota. The policy instrument used to coerce compliance with this regulation was a penalty.

4.2.2. DATA COLLECTION

Table 4.2 summarizes the parameters used to simulate the evolution of the German biodiesel supply chain (base case)[6].

Table 4.2: Techno-economic, logistic, and policy parameters

Parameter	Value	Unit	Reference
Rapeseed production cost	240 - 278	$€\,t^{-1}$	[119]
Wheat production cost	80-130	$€\,t^{-1}$	[120]
Biodiesel fixed production cost	0.08 – 0.11	$€\,l^{-1}$	[121]
Yield rapeseed oil	0.4	$kg_{oil}\,kg_{rapeseed}^{-1}$	[110]
Yield biodiesel	0.97	$kg_{biodiesel}\,kg_{oil}^{-1}$	[110]
Yield glycerol	0.11	$kg_{glycerol}\,kg_{biodiesel}^{-1}$	[110]
Yield rapeseed meal	0.56	$kg_{rapemeal}\,kg_{rapeseed}^{-1}$	[110]
Rapeseed transportation cost	0.05	$€\,t^{-1}\,km^{-1}$	[123]
Biodiesel transportation cost	3.74e-4	$€\,l^{-1}\,km^{-1}$	[123]
Premium agricultural land	301	$€\,ha^{-1}$	[122]
Premium grass land	79	$€\,ha^{-1}$	[122]
Standard agricultural premium	301	$€\,ha^{-1}$	[122]
Extra fee energy crops	45	$€\,ha^{-1}$	[122]
Tax biodiesel	0.3	$€\,l^{-1}$	[110]
Penalty	0.5	$€\,l^{-1}$	[110]
Ratio quota/total capacity	0.65	–	[96]

Table 4.3 presents the institutional chronogram used in the path dependency analysis of the liberalization of the EU agricultural market and energy tax act. The analysis is carried out using as a starting point any year in the period 1995 – 2010. It is assumed that

[6] For a more detailed overview of the data and assumptions used in the simulations the reader is referred to Moncada *et al.*[167]

the agricultural reform expires the year before the liberalization of the EU agricultural market is enacted. However, the earmarked land is only fixed to 0 % as of 2008.

Table 4.3: Institutional chronogram used in the path dependency analysis

Institution	Period	
	Starts	Expires
Agricultural reform	1992	[1994 - 2009][a]
Liberalization of the EU agricultural market	[1995 - 2010]	2015
Energy Tax act	[1995 - 2010]	2015
Biofuel quota act	2007	2015

[a] It is assumed that the agricultural reform expires one year before the liberalization of the agricultural markets is enacted.

The analysis of the impact of bioenergy policy instruments (tax, and penalty) on biodiesel production, and actor behavior is carried out based on the data presented in Table 4.4. The range of the values accounts for possible (extreme) departures from those values reported in the base case.

Table 4.4: Parameters used in both policy interaction and actor behavior analysis

Parameter	Range	Base Case	Unit
Tax biodiesel	0.2 - 1	0.3	€l^{-1}
Penalty	0.2 - 1	0.5	€l^{-1}

The analysis of the effect of actor behavior on system behavior was conducted based on the adaptation mechanism incorporated in the forecasting of prices. Agents adapt their forecasting based on the following equation [116]:

$$C_t^e = C_{t-1}^a \left(C_{t-1}^e\right)^{(1-a)} \tag{4.1}$$

where, C_{t-1}^e is the estimate for the previous year, C_{t-1} is the actual value from the past year, and C_t^e is the updated estimate for the current year. a is a parameter that weighs the influence of the actual value of the previous year as compared to the estimate in the forecasting, $0 \leq a \leq 1$.

4.3. RESULTS

4.3.1. POLICY ANALYSIS

PATH DEPENDENCE ANALYSIS

To study the effect of institutional change on the German biodiesel value chain, a path dependency analysis was carried out. The experiments were set out to explore the impact of the year of enactment of the liberalization of the EU agricultural market, and the energy tax act on biodiesel production and production capacity. The institutional chronogram used is presented in Table 4.3. Simulations were run for each permutation

100 times, and 1000 times for the analysis of the effect of timing of the introduction of liberalization of the EU agricultural market and the energy tax act, respectively.

Figure 4.4 presents the mean of biodiesel production (top) and production capacity (bottom) in the period 1992 – 2014 under different years of enactment of the liberalization of the EU agricultural market. The base case refers to the year 2003 as year of enactment of the agricultural policy. Figure 4.4 shows that the introduction of the policy prior to the year 2001 led to the stagnation of biofuel production with respect to the base case as the biodiesel market was not mature enough to compete for the feedstock. A sudden increase in biodiesel production took place upon the introduction of bioenergy policy in 2000. The production approximately matched that reported in the base case when the agricultural policy was introduced at any year of the period 2001 – 2004. As of 2005, the biodiesel production gradually decreases with reference to the base case as a late liberalization of the agricultural market inhibits its expansion. As of 2008, the biodiesel market collapsed as a consequence of the introduction of the tax in 2006 and a limited feedstock supply.

Figure 4.4 also indicates that the introduction of the policy prior to the year 2000 led to an overinvestment in production capacity. This is explained by the fact that an early liberalization of the rapeseed market increased the supply to biofuel producers. As a secure provision of feedstock is crucial in decision making about investment, an increase in the feedstock supply led to early investments. Values for production capacity roughly matched the data reported in the base case in the period 2003 – 2005. The negative effect of the tax on production capacity is enhanced when the liberalization of the agricultural market is enacted as of 2006.

Figure 4.5 presents the mean of biodiesel production (top) and production capacity (bottom) in the period 1992 – 2014 under different years of enactment of the energy tax act. The base case refers to the year 2006 as the year of enactment of the bioenergy policy. The introduction of the energy tax act prior to the year 2001 led to stagnation of biofuel production. A slight increase in biodiesel production took place when the bioenergy policy was introduced in 2002, although its production was lower than the one reported in the base case. As of 2002, production gradually increased along with the year of enactment to match the values reported in the base case in 2006. As of 2008, biodiesel production was higher than production levels reported in the base case, as a late introduction of the tax led to major investments in capacity as seen in the patterns for production capacity.

A similar pattern to that described for biodiesel production was observed for production capacity. A premature enactment of the energy tax led to stagnation. As of 2002, investment in production capacity increased. A late introduction of the tax led to major investments in capacity as it was assumed that investments in production capacity depend on the biodiesel tax. The perception that the biodiesel market will grow increases in the absence of the tax.

BIOENERGY POLICIES INSTRUMENTS INTERACTION

The experiments were set out to explore the impact of the biodiesel tax and penalty on biodiesel production and adoption of rapeseed by farmers. Permutations of the data reported in Table 4.4 were used in the simulations. 1000 simulations were carried out per each combination of parameters.

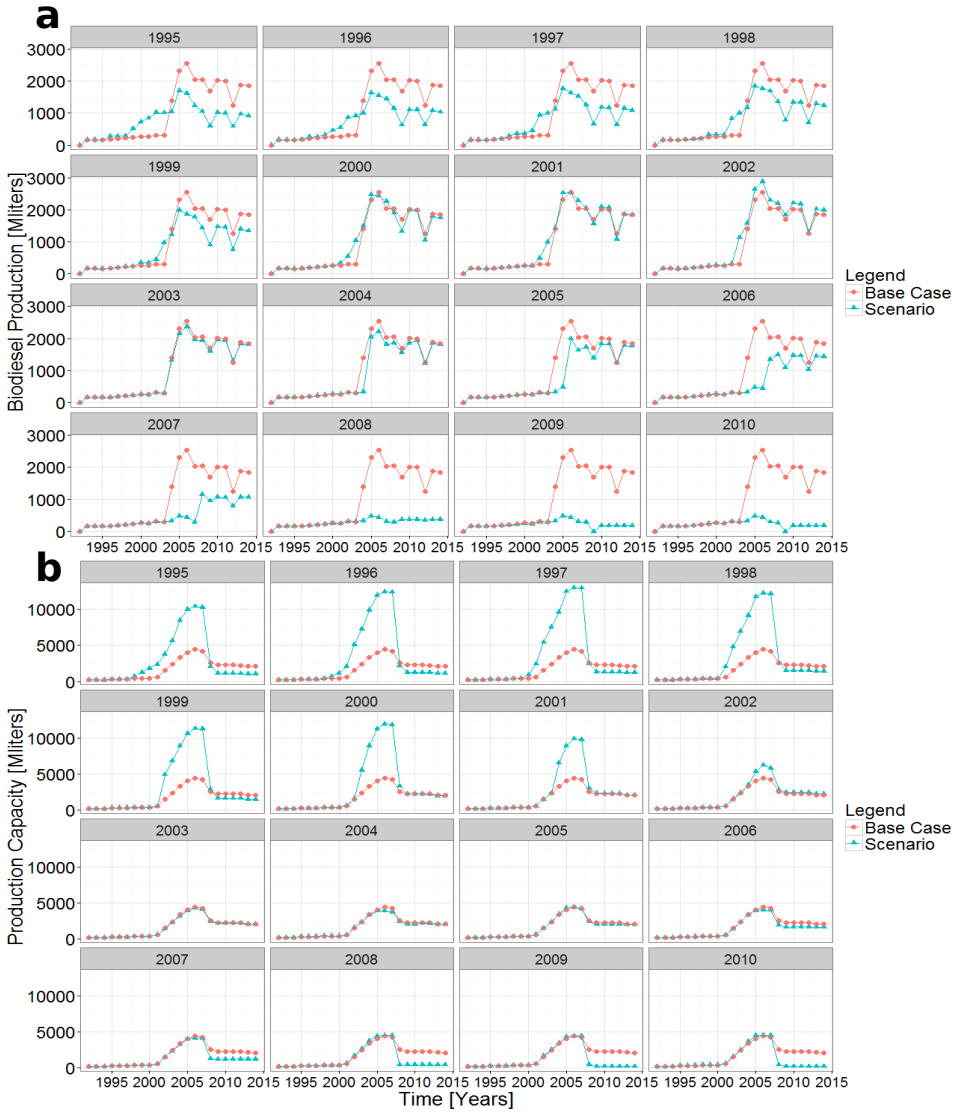

Figure 4.4: Biodiesel production (**a**) and production capacity (**b**) patterns at different years of enactment of the liberalization of the EU agricultural market.

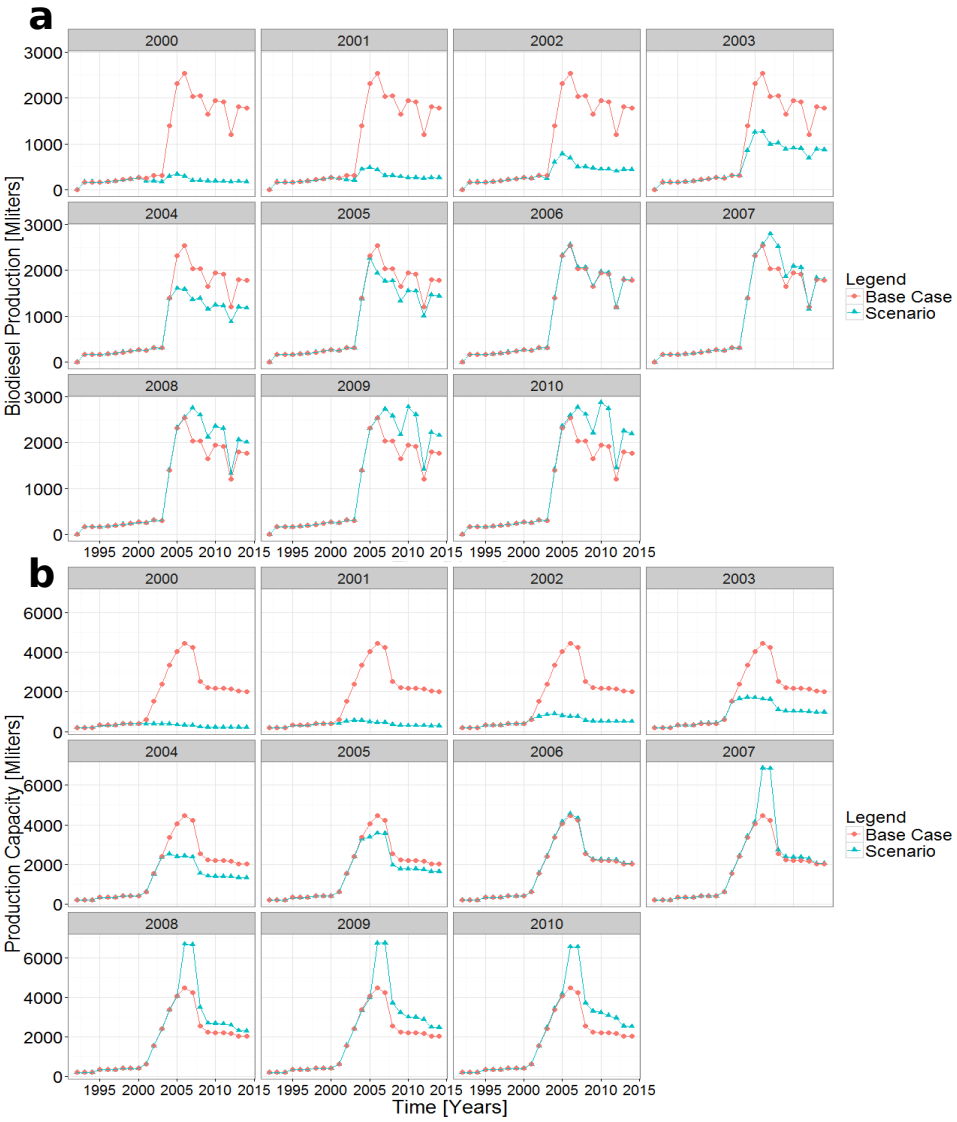

Figure 4.5: Biodiesel production (**a**) and production capacity (**b**) patterns at different years of enactment of the energy tax law.

Figure 4.6 presents biodiesel production as a function of time. The horizontal shift represents a change in the penalty for non-compliance with the biodiesel quota and the vertical shift represents a change in the tax levied on biodiesel production. These policy instruments were introduced in the biofuel quota act and energy tax act, respectively.

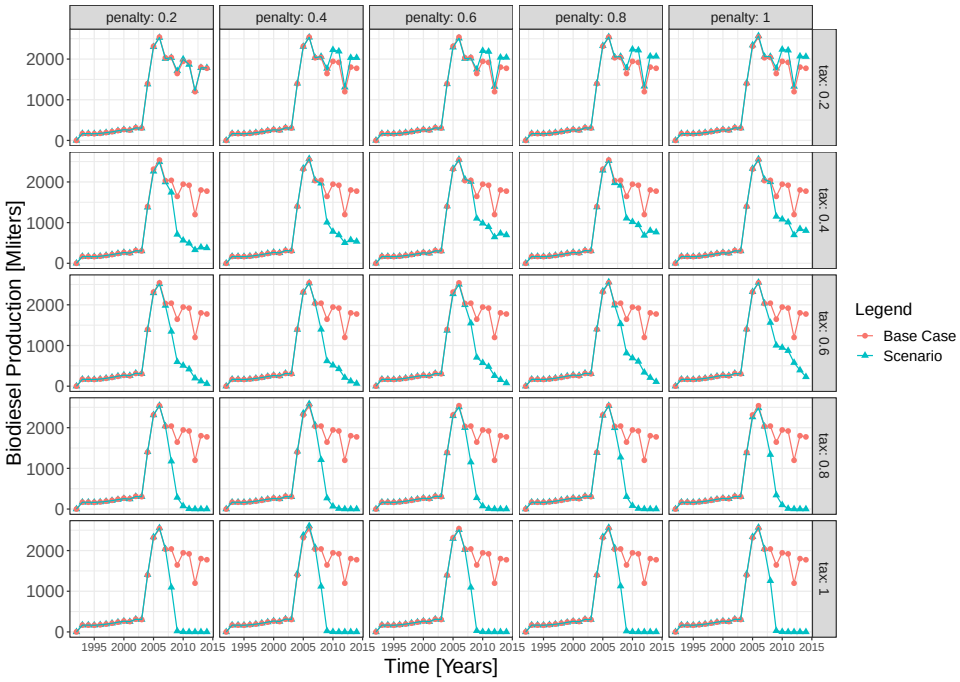

Figure 4.6: Biodiesel production as a function of time for different combinations of penalty for not producing the biodiesel quota (top) and biodiesel tax (right). Biodiesel penalty and biodiesel tax in €l^{-1}.

As shown in Figure 4.6, an increase in the value of the penalty led to an increase in biodiesel production for values of the biodiesel tax less than, or equal to, 0.6€l^{-1}. The penalty had no effect on biodiesel production for values greater than 0.6€l^{-1} for the biodiesel tax. This is due to the fact that biodiesel production is not profitable at all above this level of taxation. In contrast, biodiesel production decreased with an increase in the biodiesel tax. Overall, the effect of the biodiesel tax was greater than the penalty. This can be explained by the fact that a tax directly affects biodiesel producers whereas a penalty can be avoided. In fact, the penalty only offset the negative effect of the biodiesel tax when this tax had a value of 0.2€l^{-1}. The penalty became an effective coercive policy instrument only at lower values of taxation. For the most part, patterns in biodiesel production for different scenarios are below that reported by the base case. Values of the biodiesel tax above 0.6€l^{-1} led to a collapse in the biodiesel production.

Figure 4.7 presents the percentage of farmers adopting rapeseed as a function of time for different combinations of penalty and biodiesel tax. The horizontal shift represents a change in the penalty for non-compliance with the biodiesel quota and the vertical shift represents a change in the tax levied on biodiesel production. The figure shows that an

increase in the biodiesel tax led to lower adoption of rapeseed compared with the base case. In contrast, an increase in the penalty led to a slight increase in the adoption of rapeseed. For values of the biodiesel tax above $0.4 €l^{-1}$ the adoption of rapeseed was below of that reported in the base case at any value of the penalty. In fact, the adoption of rapeseed collapsed when the biodiesel tax was greater or equal to $0.8 €l^{-1}$.

The link between bioenergy policies and farmers' behavior arises from the introduction of the biodiesel tax in 2006 which caused the shutdown of many biodiesel production facilities leading to a decrease in the demand for rapeseed. Thus, the higher the biodiesel tax, the higher the number of plants that need to be shut down and the lower the demand for rapeseed.

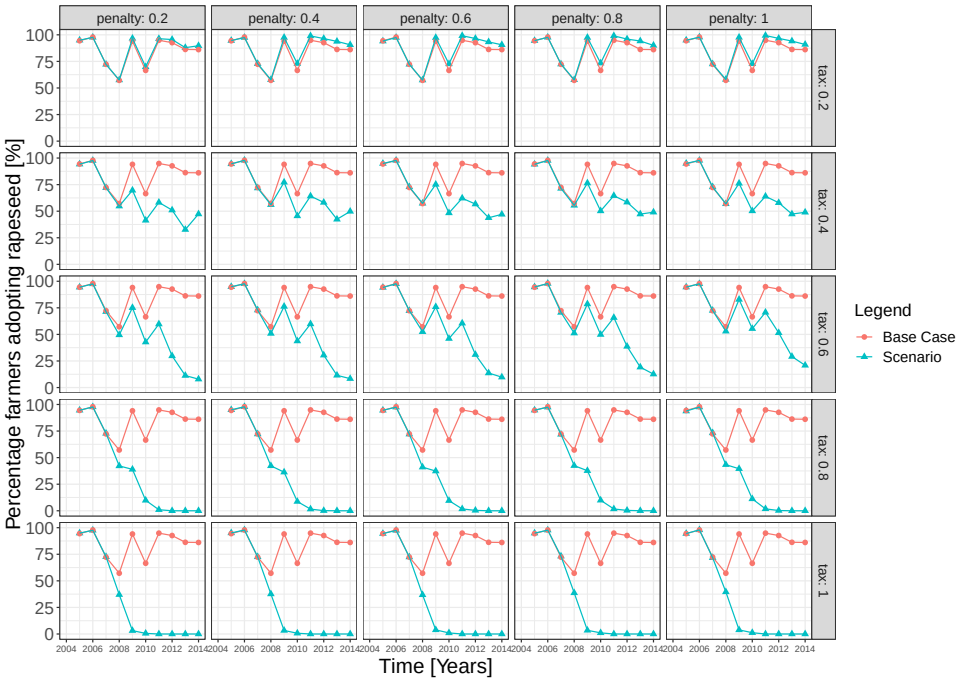

Figure 4.7: Percentage of farmers adopting rapeseed as a function of time for different combinations of penalty for not producing the biodiesel quota (top) and biodiesel tax (right). Biodiesel penalty and biodiesel tax in $€l^{-1}$.

4.3.2. EFFECT OF ACTOR BEHAVIOR ON SYSTEM BEHAVIOR.

EFFECT OF AGENTS' ADAPTATION MECHANISM TO FORECAST PRICES ON BIODIESEL PRODUCTION

Figure 4.8 shows biodiesel production patterns as a function of time at different values of the parameter a in Equation (4.1). Values of parameter a close to the unity provide a forecasting of the price that takes into account the actual price endogenously calculated in the system. That is, when the parameter a is close to unity, agents adapt their forecasting to the patterns (prices) generated in the macro-behavior. On the contrary, a value of

the parameter a close to zero implies no adaptation of the agents in their decisions. This nonadaptive behavior is due to unavailability of the information rather than lack of the intelligence of the actors. The fundamental behavioral assumption was that agents aim to improve their economic situation by making rational decisions with the information available. For the cases ($a = 0.1$; $a = 0.9$), it was assumed that all agents had the same value for this parameter.

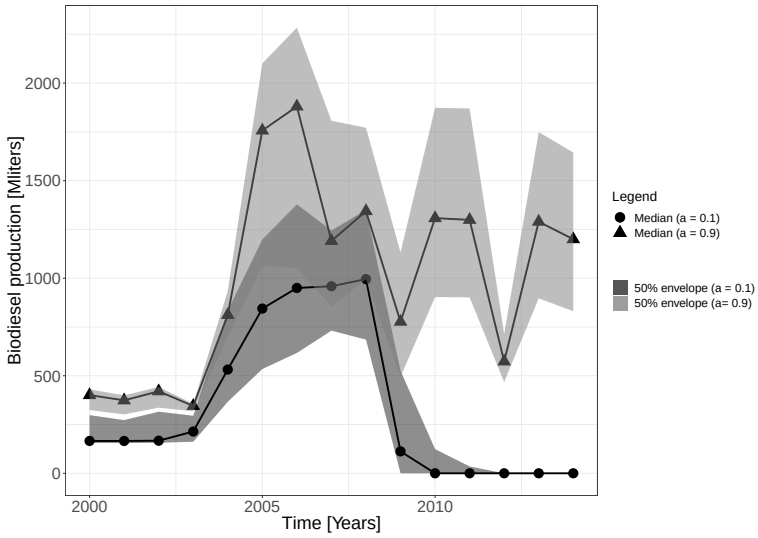

Figure 4.8: Biodiesel production as a function of time at different values of the parameter used in the forecasting of prices for rapeseed and biodiesel (see Equation (4.1))

Figure 4.8 shows that the impact of the parameter a is regime-dependent. Before the agricultural market was liberalized in 2003, the effect of the parameter on biodiesel production is negligible. However, as of 2003 biodiesel production considerably increases at higher values of the parameter a. When $a = 0.1$ biodiesel production is considerably affected; notably, after the energy tax is enacted in 2006.

The influence of the parameter a on biodiesel production can be explained by the fact that the introduction of the agricultural policy shocked the system by expanding the production of rapeseed in arable land for energy applications. An adaptation mechanism allowed agents to adapt their decision making to the new system macro-behavior. Specifically, agents expanded production of rapeseed and invested in production capacity. A similar observation can be made when the energy tax law is enacted. In general, a more limited adaptation mechanism led to lower biodiesel production.

4.4. DISCUSSION

THE results on path dependency suggest that the timing of intervention of agricultural and biofuel policies determines the evolution of the system. Model results on policy instruments interaction and actor behavior indicate that the biodiesel energy tax is the dominant policy instrument. Only the penalty could offset the negative effects of the tax

on biodiesel production and adoption of rapeseed by farmers when the latter had a low value. Finally, the results about the influence of adaptation mechanisms for forecasting prices on biodiesel production suggest that poor adaptation mechanisms caused by lack of information lead to lower biodiesel production.

The path dependence analysis of the effect of the liberalization of the EU agricultural market on biodiesel production identifies a policy window. This policy window refers to a period in which the policy should be enacted to increase the performance of the system. An execution of the agricultural policy either before or after the policy window would lead the system to an under production of biodiesel or the collapse of the biodiesel market. The formation of the policy window can be explained as follows: an early liberalization of the agricultural market would entail an increase in feedstock production as well as in the competition for feedstock. As the biodiesel market is not mature enough to compete for the feedstock with other sectors, the biodiesel production is limited. On the other hand, a late liberalization of the agricultural market inhibits the expansion of the market provided that import tariffs for rapeseed oil are too high to capture the gains from international trade.

In the case of investment in production capacity, an early introduction of the agricultural policy leads to an increase in production capacity as a consequence of the increase in rapeseed supply. The reason why investment in production capacity keeps increasing even though biodiesel production is limited, is due to the assumption that the perception of agents about expansion capacity is exclusively a function of the institutional framework. In reality, agents' perceptions about expansion capacity also co-evolve with the macro-behavior of the system (biodiesel production, prices, etc.). This model flaw could be addressed by incorporating a feedback mechanism between agents' perceptions about expansion capacity and system behavior.

The path dependence analysis of the effect of the energy tax on biodiesel production and investment in production capacity indicates, as it was expected, that an early taxation of biodiesel leads to lower biodiesel production and investment in production capacity. On the other hand, a late introduction of the tax leads to an increase in production capacity that eventually decreases as a consequence of enacting the biodiesel tax and the quota. It is important to realize that this decrease in production capacity can be utilized as a proxy for sunk costs as it is assumed that when a plant is shut down its capacity cannot be re-used. The increase in production capacity arises from the assumption that producers' expectations of sudden market growth increases in the absence of a biodiesel tax. In short, a late introduction of the tax leads to an increase in sunk costs provided that a biofuel quota is binding.

In the study of the effect of the interaction of bioenergy policy on biodiesel production, production capacity and adoption of rapeseed by farmers, two policy regimes are identified. In the first regime (biodiesel tax $< 0.3 €l^{-1}$), the penalty can offset the negative effects of the tax. Conversely, in the second regime (biodiesel tax $\geq 0.4 €l^{-1}$), the tax is the dominant policy instrument. In this regime, biodiesel production and production capacity considerably decrease.

The analysis of the effect of agents' adaptation mechanism to forecast prices on biodiesel production suggests that system performance depends on the ability of agents to adapt to it in the event that an external shock (the introduction of a new policy) is in-

troduced in the system. As pointed out by Arthur: *"behavior creates pattern; and pattern in turn influences behavior"* [74]. This interplay between the micro-system (individual behavior) and the macro-system (system behavior) has been recognized by economists since Adam Smith. Unlike an optimization approach, this feedback mechanism can be incorporated in agent-based models as demonstrated in this study.

The analysis carried out in this study extends the literature on path dependency, where analysis has been limited to qualitative analysis of historical case studies, by incorporating a quantitative analysis. Moreover, this study extends the analysis done by Kaup & Selbmann [96] by identifying different policy regimes with their respective dominant policy instruments, and by shedding light on new mechanisms that drive the behavior of the system such as the co-evolution between individual behavior and system behavior. Understanding the path dependency of different policy interventions and identifying their policy regimes with their respective dominant policy instruments on existing biofuel supply chains might provide insights on how to efficiently develop new biofuel supply chains such as bio jet fuel supply chains.

The study neglects organizational structures of farmers and biofuel producers. Future research should explore the effect of policies on organizational structures. These structures can have a considerable effect in the performance of the system as they determine the transaction costs. An increase in the transaction costs might reduce the amount of capital available to invest.

Still, the analysis carried out in this study should give more evidence of the potential application of agent-based modelling (ABM) in the analysis of (bio) energy systems. Unlike conventional models, ABM allows the exploration of actor behavior as a function of different policy interventions, the incorporation of feedback mechanisms (adaptation), and allows a more realistic description of the actors and their decision making (bounded rationality). Even further, ABM can be used along with optimization approaches to assess what policy strategies are more effective in leading the system to its optimum and to explain what mechanisms play an important role.

4.5. CONCLUSIONS

THE study was conducted to answer the following research question: *What patterns in biodiesel production and production capacity are generated as a result of applying different policy interventions in Germany in the period* 1992 - 2014*?* To answer that question, an agent-based model was developed. The model was used to explore the impact of the timing of the enactment of specific agricultural and bioenergy policies (path dependence) on patterns in biodiesel production and production capacity. The model was also used to analyze the impact of policy instruments such as biodiesel tax and penalty on patterns in biodiesel production and adoption of rapeseed by farmers. Finally, the influence of agents' adaptation mechanisms to forecast prices on patterns in biodiesel production was studied.

Based on the path dependency analysis, we find that the timing of intervention of agricultural and biofuel policies determines the evolution of the system. An early (late) liberalization of the agricultural market leads to a under production of biodiesel (collapse of the market). Hence, to stimulate production of biodiesel, the agricultural market should be enacted within a policy window. On the other hand, an early introduction of

the biodiesel tax leads to stagnation in biodiesel production and investment in production capacity. A late introduction of the tax leads to an increase in sunk costs provided that the biofuel quota is binding.

Considering the results of the interaction of bioenergy policy instruments, we argue that patterns in biodiesel production and rapeseed adoption depend on the policy regime and its dominant policy instrument. When the biodiesel tax is the dominant policy instrument biodiesel production and rapeseed adoption patterns decrease following an increase in the level of taxation. This negative effect can be offset by the penalty only if the biodiesel tax is not dominant.

In light of the analysis of the effect of agents' adaptation mechanism to forecast prices on biodiesel production, we argue that poor adaptation mechanisms caused by lack of information lead to a decrease in biodiesel production upon introduction of an external shock to the system. The implications of this insight are twofold. First, it gives evidence that system behavior is influenced by individual behavior. Second, the unstable nature of the institutional framework to stimulate the production and consumption of bioenergy, the limited information available, and the limited processing information capacity of the actors, point to the need for mechanisms that improve the accessibility of pertinent information to the agents. One alternative could be to increase the transparency in trade statistics for both agricultural and bioenergy markets.

The insights of this study might underpin policy making for the creation of new biofuel supply chains. A better understanding of the role of institutions on existing biofuel supply chains might accelerate the implementation of new biofuel supply chains, such as the biojet fuel supply chain, in other countries.

Given these points, we argue that the incorporation of the influence of institutions on the performance of bioenergy systems should be a fundamental part of the research agenda. Institutions influence behavior, which in turn determines the properties of the system. Unlike optimization approaches, agent-based modelling is suitable to incorporate these types of feedback mechanisms as this study has demonstrated. Particularly, it is of interest to analyze the co-evolution of formal institutions (policies) and system behavior. That issue will be the subject of analysis in future work.

5

INSTITUTIONAL ANALYSIS OF THE BRAZILIAN ETHANOL SUPPLY CHAIN

A system is a big black box
Of which we can't unlock the locks,
And all we can find out about
Is what goes in and what comes out.
Perceiving input-output pairs,
Related by parameters,
Permits us, sometimes, to relate
An input, output and a state.
If this relation's good and stable
Then to predict we may be able,
But if this fails us - heaven forbid!
We'll be compelled to force the lid.

Kenneth Boulding, *General Systems as a Point of View*

This chapter has been published as Moncada, J.A., *et al.*, Exploring policy options to spur the expansion of ethanol production and consumption in Brazil: an agent-based modelling approach. Energy Policy, 2018. 123: p. 619-641.

The Brazilian government aims to increase the share of biofuels in the energy mix to around 18% *by* 2030, *which implies an increase of ethanol production from currently* 27 *bln liters to over* 50 *bln liters per year. Biofuel policies play an important role in ethanol production, consumption, and investment in processing capacity. Nevertheless, a clear understanding of how current policies affect the evolution of the market is lacking. We developed a spatially-explicit agent-based model to analyze the impact of different blend mandates and taxes levied on gasoline, hydrous, and anhydrous ethanol on investment in processing capacity and on production and consumption of ethanol. The model uses land use projections by the PCRaster Land Use Change model and incorporates the institutions governing the actors' strategic decision making with regard to production and consumption of ethanol, and the institutions governing the interaction among actors. From the investigated mix of policy measures, we find that an increase of the gasoline tax leads to the highest increased investments in sugarcane processing capacity. We also find that a gasoline tax above* 1.23 $\mathrm{R\$\,l^{-1}}$ *and a tax exemption for hydrous ethanol may lead to doubling the production of ethanol by* 2030 *(relative to* 2016*).*

5.1. INTRODUCTION

DURING the 2015 United Nations climate conference in Paris, Brazil indicated that bioenergy will significantly contribute towards their realization of climate objectives. The Brazilian government aims to increase the share of biofuels in the energy mix to around 18% by 2030 [11], which implies that ethanol demand will increase from 27 bln liters per year in 2016 to more than 50 bln liters in 2030 [169]. If this projected demand for ethanol is to be met by domestic supply, it would be necessary to double the production of ethanol in the next years. It is expected that over 70% of the increase in ethanol supply is to be met by hydrous ethanol because of the technical blend constraints of anhydrous ethanol in the fuel market [170]. Nevertheless, the feasibility of achieving this increase in ethanol supply with the current set of policies is unclear. The effect of existing Brazilian policies on the evolution of the ethanol market is not well understood [171].

The Brazilian experience with biofuels dates back to the early part of the last century. Nevertheless, it was not until the global crisis in 1970 that the Brazilian government initiated the large scale implementation of ethanol in Brazil with the ProAlcool program [172]. Since then, Brazil has become the world's top producer of sugar and, until 2005, the top producer of ethanol. Nowadays, Brazil has the second largest production of ethanol after the U.S. [173]. Key success factors of the Brazilian ethanol market are the favorable environmental conditions, technological innovations, and the governmental policy [174].

On the technical side, technological innovations such as flex plants and flex vehicles are at the core of the ethanol market structure. Flex plants can produce flexible ratios of sugar and ethanol from sugarcane [175]. Based on the water content, ethanol can be classified as: hydrous ethanol (up to 4.9% v/v of water) and anhydrous ethanol (up to 0.4% v/v of water). Users of flex vehicles can switch back and forth from E100 (hydrous ethanol) to gasohol (a blend of gasoline and anhydrous ethanol, of which the max share of anhydrous ethanol is 27.5% v/v due to technical limitations) [176]. Indeed, this flexibility at both the supply and the demand side of the market is one of the factors responsible for the success of ethanol in Brazil [177].

On the policy side, the governmental ethanol policy has undergone many changes [174]. The ProAlcool program had different phases (creation, consolidation, expansion, and political uncertainty) with different characteristics [172]. The period 1979-1985 was marked by strong state intervention, whereas the sugar and ethanol industry were deregulated in the 1990s. In this period subsidies and regulation were gradually removed [178]. The revitalization of the ethanol market was triggered by the introduction of the flex vehicle in 2003 [179].

The behavior of the Brazilian ethanol market is shaped by both governance structures and policy instruments. The interaction between farmers and mill/distillery owners is governed by the Conselho de Produtores de Cana-de-Açúcar, Açúcar e Etanol do Estado de São Paulo (CONSECANA-SP) mechanism. In this governance structure, the sugarcane price is determined by two factors: the amount of total recoverable sugar (TRS) in the sugarcane and the prices of sugar and ethanol on the domestic and foreign markets [180]. Policy instruments such as blend mandates, and taxes levied on gasoline, hydrous, and anhydrous ethanol influence patterns of demand and production of ethanol. For instance, when the government increased the CIDE (Contribution for Inter-

vention in the Economic Domain) tax for gasoline in 2015, ethanol demand and production increased [181]. These instruments and their interaction produce distortions in the ethanol market that might shape both the development of the ethanol industry [34, 182], and the share of biofuels in energy consumption.

The understanding of the effect of policies on the ethanol market is still limited. Analyses have been carried out to shed light on the effects of U.S. policies on Brazilian markets [183, 184], on the ethanol-sugar-oil nexus [185], on the effects of blending targets around the world on sugarcane demand in Brazil [25, 186] and on the effects of Brazilian policies on ethanol markets [34, 171, 187, 188].

Studies using a structural economic model of the Brazilian ethanol market include Dabrik *et al.* [187] and Demczuk *et al.* [34]. The mathematical model of Dabrik *et al.* indicated that a low gasoline tax and a high tax exemption for anhydrous ethanol lead to a reduction in both ethanol and sugar prices. Nevertheless, this model neglected the effect of institutions at two levels. First, at the level of decision making, the profit maximizing behavior by the flex plants that determines the production of ethanol and sugar was not included. Although the authors did take into account the shift in demand curves from E100 to gasohol, this mechanism was imposed on the model. In reality, consumption patterns for both fuels emerge as a result of the strategic behavior of the flex vehicle users [176]. Second, at the level of governance structures, the model neglected the CONSECANA-SP mechanism that determines the sugarcane price.

Demczuk *et al.* [34] developed a system dynamic model to analyze the effect of Brazilian policies on the development of the ethanol industry. The authors argued that the liberalization of the gasoline prices and the homogenization of sales taxes on ethanol among the Brazilian states could reduce uncertainty in the ethanol sector, and thus encourage investments in technology and production capacity. This modeling study incorporated the CONSECANA-SP mechanism, but it neglected the profit maximizing behavior by the flex plants and the arbitrage in the consumption of gasohol and hydrous ethanol by the flex vehicle users, as well as the diversity among flex plants (e.g. they do not produce the same sugar to ethanol ratio under the same market prices) and among the flex vehicle users (e.g. they do not all consume the same fuel given the same fuel prices).

In this study, we developed a spatially-explicit agent-based model of the Brazilian ethanol/sugar market to explore the effect of biofuel policies on the market behavior. The model accounts for the institutions governing the actors' strategic decision making with regard to production of ethanol by including the profit maximization behavior of the flex plants; the consumption of ethanol by including the arbitrage behavior of the users of the flex vehicles; and the investment in processing capacity of sugarcane. The model is spatially explicit to account for the influence of the location of the sugarcane fields and their availability on the decision of investment in sugarcane processing capacity. The agent-based model uses land use projections provided by the PCRaster Land Use Change (PLUC) model [189] to explicitly account for expansion of land for sugarcane production in specific locations. The agent-based model also accounts for the interaction among actors by incorporating the CONSECANA-SP and supply and demand mechanisms; for the diversity among actors by including differences in the preferences in the consumption of ethanol of flex vehicles users, and differences in the production

ratio of sugar and ethanol of flex plants. In particular, the model is used to shed light on the following research question:

- What is the combined effect of different options for blend mandate and tax levied on gasoline, hydrous, and anhydrous ethanol on the development of the sugarcane-ethanol market in Brazil?

We focus only on sugarcane-ethanol (1st generation ethanol[1]) as it is projected that the highest share in the production of ethanol in the period 2017-2030 will come from sugarcane-ethanol. According to Tolmasquim *et al.* [170], 2nd generation ethanol[2] will emerge in considerable volumes as of 2023, reaching 2.5 billion liters in 2030.

The chapter is organized as follows: Section 5.2 provides a description of the concepts underpinning the model structure, an explanation of the developed agent-based model, and the data used. The results are presented in Section 5.3, followed by a discussion in Section 5.4. Finally, conclusions are drawn in Section 5.5.

5.2. THEORY AND METHODS

THIS section describes the methodological improvements performed and considered crucial for modeling the ethanol market in Brazil.

5.2.1. SYSTEM DIAGRAM AND CONCEPTUAL FRAMEWORK

Figure 5.1 shows a system diagram of the Brazilian ethanol/sugar market. The system is analysed from the perspective of the Brazilian government. It is assumed that the Brazilian government aims to increase the share of ethanol in the energy matrix as well as encourage expansion in sugarcane processing capacity of flex plants. While the government has used policy instruments to spur the production and consumption of ethanol such as investments in RD&D in universities and research centers, subsidies to metallurgic industries and farmers, fiscal policies (tax levied on gasoline, hydrous, and anhydrous ethanol), and blend mandates, we focus on fiscal policies and blend mandates. It is assumed that the behaviour of the system is driven by a number of external factors as depicted in Figure 5.1.

The Brazilian ethanol market is a complex adaptive system. It consists of heterogeneous actors (farmers, ethanol/sugar producers, distributors, and end-users) interacting in a dynamic environment and regulatory regime. Actors constantly adapt their behavior to changing market prices and available supply of ethanol and sugar. Producers adjust their production ratio between ethanol and sugar in accordance to their own specific market expectation. Flex vehicle users switch from E100 to gasohol if a significant increase in ethanol prices occurs, and switch back in case of a decrease.

The system was conceptualized based on the tenet that an adequate representation of a complex system stems from the integration of knowledge of various domains and disciplines [48]. The conceptual framework proposed by Moncada *et al.* [167] was chosen as a starting point for analysis as it has been successfully used in the analysis of

[1] 1st generation ethanol refers to the ethanol that has been derived from edible sources such as corn, starch, and sugarcane.

[2] 2nd generation ethanol refers to the ethanol that has been derived from non-food biomass such as lignocellulosic biomass, agricultural residues or waste, and non-food energy crops.

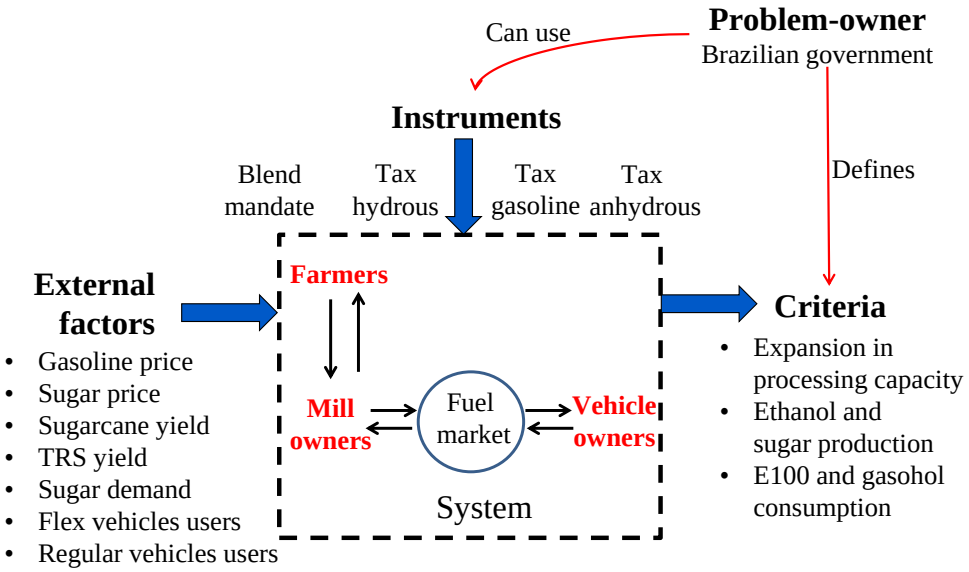

Figure 5.1: System diagram with interacting actors of the Brazilian ethanol market

how institutions affect the evolution of biofuel supply chains in Germany [190]. The basic principle of the framework assumes that the behavior of the complex socio-technical system is the result of the interaction of three elements: the physical system, the network of actors, and institutions (see Figure 5.2).

The physical system refers to the physical objects such as: farms, mills/distilleries, and vehicles. The actors are the entities that make decisions such as: farmers, mills/distillery owners, and end-users (car owners). Finally, institutions are the rules that shape actors' behavior. Examples of institutions are: norms, regulations, technical and operational standards, legislation, policies, governance structures, and traditions [73].

Institutions interact with the network of actors at different levels. At the level of one single actor, institutions (i.e. games) refer to the rules, norms and shared strategies of individuals within an organization. In the Brazilian ethanol market, the selection of a production ratio for sugar/ethanol by refineries accounts for the interaction between institutions and actor at this level. At one level of analysis higher (i.e. institutional arrangements), institutions describe how different actors interact. Usually, this interaction is carried through by three mechanisms: spot market, bilateral contracts, and vertical integration. In this study, the interaction between farmers and mills/distillery owners is governed by the CONSECANA-SP mechanism. At the same level of analysis, it was assumed that the interaction between mills and car drivers is governed by a supply-demand mechanism. That is, the price and quantity of the fuels to be traded are determined by the intersection of the supply and demand curves. In reality, however, distribution companies and gas stations owners are responsible for a significant share of the final prices because of cartel practices. At the highest level of analysis (i.e. formal institutional environment), institutions refer to the rules of the game. The blending

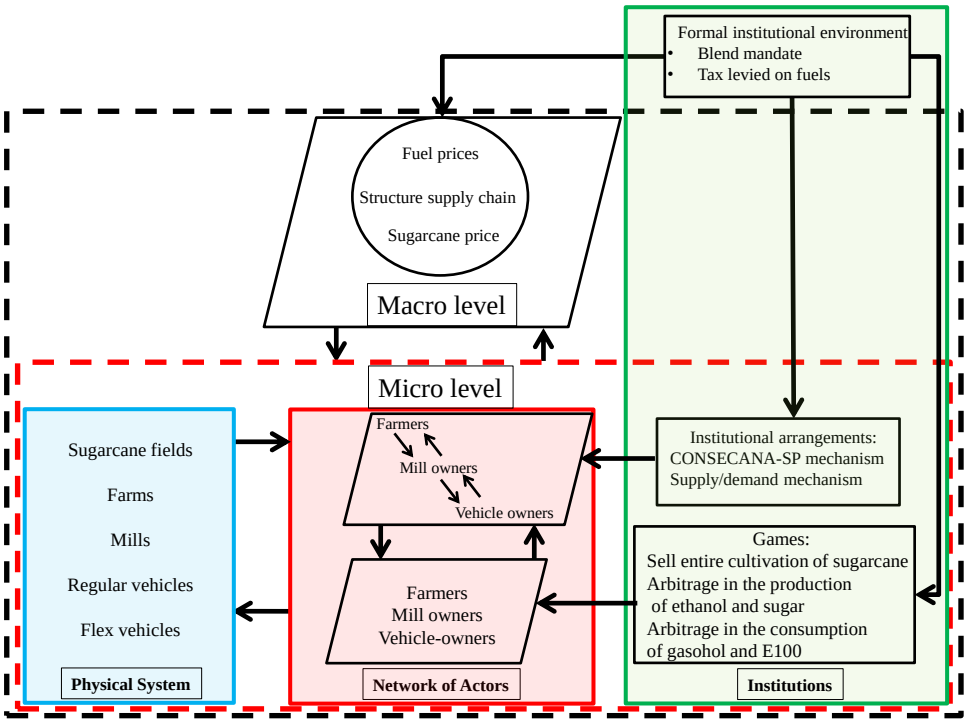

Figure 5.2: Conceptual framework adapted from Moncada *et al* [167]. The dashed black box line represents the system boundaries. The dashed red box line separates the micro level from the macro level.

mandate, tax exemptions, and the promotion of flex vehicles are examples of institutions in the Brazilian ethanol market. At this level, institutions are assumed to be exogenous. We focus our analysis on the effect of the blend mandate and taxes levied on gasoline, hydrous and anhydrous ethanol on the development of the sugarcane-ethanol market.

The theories used to describe the interaction among different building blocks are: complex adaptive systems (CAS), and rational choice theory. CAS is used to describe how the macro behavior of the system emerges as a result of the interactions among different system components and how, in turn, these components adapt to the macro behavior they created [191]. Rational choice theory is used to describe the decision making of mill owners and flex vehicle owners with regard to the production and consumption of ethanol, respectively [192].

Supported by these theories, the conceptual framework is formalized into an agent-based model to analyze the influence of formal institutions on the evolution of the Brazilian sugarcane ethanol market. Agent-based modeling (ABM) was chosen as a modeling paradigm for its explicit bottom-up approach, easiness of including the effect of preferences on actors' decision making, the actors' diversity, and actors' adaptive behavior. These are necessary elements to describe a complex adaptive system such as the Brazilian ethanol market. These elements have been neglected by previous stud-

ies [34, 171, 187]. Applications of ABMs in the analysis of socio-technical systems vary from economics [50, 99, 100, 193] to energy systems [53, 54, 103–105] and supply chains [106, 107].

5.2.2. MODELING FRAMEWORK

The modeling framework consists of two building blocks: the PCRaster Land Use Change model (PLUC) and the agent-based model of the Brazilian sugar-ethanol market. PLUC is a spatial explicit land use change model that stochastically projects annual land use maps [194]. In a previous study, it has been applied to Brazil, for which it projects the expansion and contraction of 11 different land use types between 2012 and 2030 at a 5 x 5 km resolution [189]. As sugarcane is one of the 11 land use types, this study provides us with annual probability maps of the occurrence of sugarcane fields from 2012 to 2030. This information is supplied to the agent-based model of the Brazilian market to model the expansion in the production of sugarcane. It is assumed that this process of expansion is driven by an increase in the demand for sugar or ethanol.

The structure of the agent-based model was designed using the pattern-oriented-modeling approach [168]. Three patterns guided the design: flexibility in the production of ethanol and sugar, flexibility in the consumption of ethanol, and the location of sugarcane availability. The model is spatially-explicit as the sugar market is local, decentralized, and land for expansion is limited. The following description of the agent-based model is based on the ODD (Overview, Design concepts, and Details) protocol proposed by Grimm *et al* [195]. The model was implemented in NetLogo [124] along with the R extension of NetLogo [196].

Purpose: the aim of the model is to study the influence of various policy instruments on the expansion of the Brazilian sugarcane ethanol market. Unlike previous thinking about the Brazilian ethanol market [34, 171, 187], this model takes a bottom-up approach. The impact of policies on both actors' preferences for production and consumption of ethanol, and actors' interactions is explicitly modeled.

A hallmark of the Brazilian ethanol market is its flexibility in both production and consumption of ethanol. The mapping between policies and actor behavior leads to a better description of the flexibility of the ethanol market, which is the result of the aggregation of actors' decision making on production and consumption of ethanol.

Entities, state variables and scales: The entities in the model are the actors in the supply chain. Actors, contrary to traditional economic analysis, behave based on their own local information (i.e. actors have bounded rationality). Farmers, mills/distillery owners, and drivers are the actors considered in our analysis of the ethanol-market. Farmers perform the role of sugarcane producers and suppliers; the main farmers' state variables are: farm area, sugarcane yield, and TRS yield. Mills/distillery owners perform the role of sugar and ethanol producers and suppliers; the main mills/distillery owners' state variables are: type (flex plant, sugar plant, and ethanol plant), sugarcane processing capacity, production costs, and production ratio of sugar and ethanol. Vehicle owners perform the role of fuel consumers; main vehicle owners' state variables are: vehicle type

(flex vehicle[3], regular vehicle[4]), energy demand, and preferences in the consumption of fuels. Farmers and mills are modeled spatially explicitly, whereas drivers are not. This is because we assumed that E100 and gasohol prices are uniform over space. The global environment consists of the policy instruments (blend mandate, taxes on gasoline, hydrous, and anhydrous ethanol), and the exogenous factors (annual world market prices of sugar and gasoline, number of flex and gasohol vehicles, sugar demand, and sugarcane and TSR content yield). The temporal extent of the model is 18 years (2013-2030) and the time step is one year. The model is spatially explicit, covering the whole of Brazil. The PLUC input has a resolution of 5 x 5 km.

Process overview and scheduling: the scheduling is formed by a set of events that take place sequentially in discrete periods within a year. During harvest season, farmers *harvest sugarcane, negotiate* with the mills agents about price and quantity to be traded and *deliver the sugarcane* to the mill as it was agreed. These transactions are decentralized and take place at different locations. The interaction between farmers and mills agents is bound to their spatial location. Mills only interact with farmers within a radius of up to 50 km [197].

Mills/distillery owners store the sugarcane and maximize profits *by deciding on volumes of sugar, hydrous and anhydrous ethanol to be produced*. In each time period, Mills/distillery owners *produce* sugar and ethanol and *ask prices and quantities to the sugar and fuel markets*. Drivers *choose* between E100 and gasohol based on relative prices. According to the market outlook, mills agents *decide about the expansion of the sugarcane processing capacity*. The new sugarcane processing capacity starts operation at the third year of construction.

Design concepts: the concepts underpinning the design of the agent-based model are presented below.

Basic principle: The basic principle applied in the model is the rational choice theory. This theory is used to describe the decision making on production of sugar and ethanol, and consumption of gasohol and E100. Nevertheless, unlike previous studies [34, 171, 187], this model incorporates the influence of diversity in preferences in the decision making process.

Emergence: Emergent system dynamics includes gasohol and E100 prices, total production of sugar and ethanol, total demand for gasohol and E100, and the expansion of the processing capacity of sugarcane.

Adaptation: Flex mill owners and the drivers of flex vehicles are the entities that exhibit adaptive behavior in the model. Owners of flex mills adapt their production ratios of ethanol/sugar based on market signals (see Figure 5.3). This behavior is driven by a profit maximization strategy. Thus, high prices of sugar (ethanol) lead to an increase in the production of sugar (ethanol).

[3] Flex vehicles can run in any combination of E100 (hydrous ethanol) with gasohol (blend of gasoline and anhydrous ethanol)

[4] Regular vehicles can only run with gasohol.

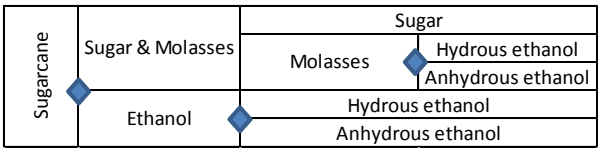

Figure 5.3: Levels of decision as to production of sugar, hydrous, and anhydrous ethanol. Each rhomboid represents a level of decision making in the model.

The decision of the flex mills about the volumes of sugar and ethanol to be produced is modeled as an optimization problem as presented below:

$$\underset{x_s, x_h, x_{hm}}{\text{maximize}} \quad \sum_{i=1}^{3} \pi_i \tag{5.1a}$$

$$\text{subject to} \quad x_s >= x_{s_{min}} \tag{5.1b}$$

$$x_s <= 0.65 \tag{5.1c}$$

$$x_h >= 0.2 \tag{5.1d}$$

$$x_h <= x_{h_{max}} \tag{5.1e}$$

$$x_{hm} >= 0.2 \tag{5.1f}$$

$$x_{hm} <= x_{h_{max}} \tag{5.1g}$$

where π_i is the profit derived from product i (sugar, hydrous, and anhydrous), x_s is the ratio of sugar production to sugarcane processed (the rest is used for ethanol production), x_h is the ratio of hydrous production to total ethanol production from sugarcane (the rest is anhydrous), x_{hm} is the ratio of hydrous production to total ethanol production from molasses. $x_{s_{min}}$ is the minimum in the ratio of sugar production to sugarcane processed, $x_{h_{max}}$ is the maximum in the ratio of hydrous production to total ethanol production. Values for $x_{s_{min}}$ and $x_{h_{max}}$ differ among mills. These values were obtained from a uniform distribution $x_{s_{min}} \in U(a,b)$ and $x_{h_{max}} \in U(c,d)$ for sugar and hydrous ethanol, respectively. The intervals of the uniform distribution are determined in the calibration of the model (see Appendix D).

To account for the influence of policy instruments (i.e. gasoline tax) on the decision making about the volumes of hydrous and anhydrous ethanol to be produced, it was assumed that the values in Equation (5.1e) and Equation (5.1g) are estimated based on the variation of the gasoline tax with respect to the value of the gasoline tax used in the model calibration[5].

$$\Delta t_G = t_G - t_{G_{bs}} \tag{5.2}$$

[5]Equation (5.3) was derived based on the assumption that owners of flex plants will only produce hydrous ethanol when the gasoline tax increases to 2.46 R1^{-1}

$$\Delta x = \frac{\left(\frac{\Delta t_G}{0.22} \cdot 10\right)}{100} \tag{5.3}$$

$$x_{h_{max}} = x_{h_{max}} + \Delta x \tag{5.4}$$

where:

Δt_G: difference in the gasoline tax with respect to the baseline.

t_G: gasoline tax.

$t_{G_{bs}}$: gasoline tax in the baseline.

Δx: difference in the maximum production ratio of hydrous with respect to the baseline.

Drivers of flex vehicles react to price signals and change from one fuel to the other on a daily basis, for this type of vehicles can use either ethanol or gasoline. The criterion for choosing ethanol (E100) as opposed to gasoline is:

$$\frac{P_{ethanol}}{P_{gasoline}} <= T_c \tag{5.5}$$

Where T_c is the drivers' preference of the relative price between E100 and gasoline. $P_{ethanol}$ and $P_{gasoline}$ are the prices for ethanol and gasoline, respectively. On average, E100 is considered to deliver 70% of the mileage of gasoline for the same volume of fuel. Thus, according to classical economic theory, $T_c = 0.7$, whereas in our model $T_c = N(m, 0.1)$ to account for the fact that some drivers have a preference for the consumption of ethanol even when this is not the optimal choice [176]. The mean of the normal distribution (m) is calibrated (see Appendix D). Strategic behavior of drivers as to buying gasohol/flex vehicles was neglected. The scope of the model as to drivers' decision making was limited to the choice of the consumption of fuels.

Objectives: Flex mill owners are profit maximizing agents. They aim to maximize their profits by shifting the production ratio of sugar to ethanol. The production ratio is a measure of the sugarcane used to produce sugar and ethanol. A technical constraint is that this ratio has to be between 35 percent and 65 percent [117]. Drivers of flex vehicles aim to meet their energy demand by choosing between gasohol and E100. Farmers aim to sell their entire sugarcane cultivation to the owners of flex/distillery plants.

Learning/prediction: Mills forecast prices and demand for sugar and ethanol (hydrous and anhydrous). The method used for forecasting is the double exponential smoothing[6] [198]. The forecasting is used to inform the decision making as to whether to invest

[6]The double exponential smoothing is a forecasting method. The forecast value at any time is a function of all the available previous values. Nevertheless, recent observations are given relatively more weight in

in a new flex plant or not. Agents lack any learning mechanisms.

Sensing: Farmers, owners of mills/distilleries and drivers are assumed to know, without uncertainty, the global variables (i.e., market prices).

Interaction: Farmers directly interact with owners of mills/distilleries in their neighborhood through the negotiation about a contract for the supply of sugarcane. The main issue in the contract is the sugarcane price. This interaction is modeled through the CONSECANA-SP mechanism. Mills interact indirectly with neighboring mills by competing for contracts with farmers in their common sourcing region in the sugarcane market.

In the CONSECANA-SP mechanism the pricing of sugarcane is based on two variables: the amount of total recoverable sugar (TRS), which expresses the sugar content that is used for sugar and ethanol production, and the price of TRS. Values of (TRS) per ton of sugarcane are given to the farmer agents.

The TRS price is linked to the average market selling prices of three different products (sugar, hydrous and anhydrous ethanol), over the period of one harvest season. The CONSECANA-SP model then assumes that sugarcane accounts for 59.5% of the production costs of sugar, and accounts for 62.1% of ethanol production [180]. Thus, remuneration to suppliers is done according to these percentages.

$$P_s^{TRS} = \frac{0.595 P_s^{ave}}{sc_s} \tag{5.6}$$

$$P_h^{TRS} = \frac{0.621 P_h^{ave}}{sc_h} \tag{5.7}$$

$$P_a^{TRS} = \frac{0.621 P_a^{ave}}{sc_a} \tag{5.8}$$

where P_s^{TRS}, P_h^{TRS}, and P_a^{TRS} are the TRS prices for sugar, hydrous ethanol, and anhydrous ethanol, respectively, in Reais per kilogram of TRS. P_s^{ave},P_h^{ave}, and P_a^{ave} are the average market selling prices for sugar, hydrous ethanol, and anhydrous ethanol in Reais per kilogram of sugar and Reais per litre of ethanol, respectively. sc_s, sc_h, and sc_a are the stoichiometric coefficient for sugar, hydrous ethanol, and anhydrous ethanol, respectively.

Nevertheless, the TRS price is unique for each processing plant as sugar sales and ethanol sales volumes differ depending on the production ratios of each processing facility. The TRS price for a processing plant i is based on weighing the product TRS price with the volumes of each product:

$$P_i^{TRS} = P_s^{TRS} \frac{Pr_s}{Pr_t} + P_h^{TRS} \frac{Pr_h}{Pr_t} + P_a^{TRS} \frac{Pr_a}{Pr_t} \tag{5.9}$$

$$Pr_t = Pr_s + Pr_h + Pr_a \tag{5.10}$$

forecasting than the older observations. Unlike the simple exponential smoothing, the double exponential smoothing adds a growth factor to the equation to account for changes in the trend.

Where P_i^{TRS} is the TRS price of the plant i in Reais per kg of TRS. Pr_s, Pr_h, and Pr_a are the total production of sugar, hydrous ethanol, and anhydrous ethanol of the plant i, respectively in kilograms of TRS.

The interaction between mills and drivers is mediated via the fuel market. The concept of preference of the relative price between E100 and gasoline is at the core of the modeling of the fuel market. Let Q_g^0, and Q_e^0, be the initial demand (measured in GEELS[7]) of gasohol and E100, respectively. Let P_g^0, and P_e^0 be the initial market prices calculated at values of demand of gasohol and E100, respectively. When the price gap between gasohol and E100 narrows, some flex car owners who previously preferred hydrous ethanol will find it attractive to switch to the blended fuel. In this case, the demand for gasohol increases to Q_g^1 whereas the demand for E100 decreases to Q_e^1. This change in demand for fuels affects the relative price as new values for the market prices are determined (P_g^1, P_e^1). This iterative process continues until the relative price remains constant (i.e. the equilibrium is reached). This mechanism is shown in Figure 5.4. The equilibrium is described by the pairs (Q_g^*, P_g^*),(Q_e^*, P_e^*).

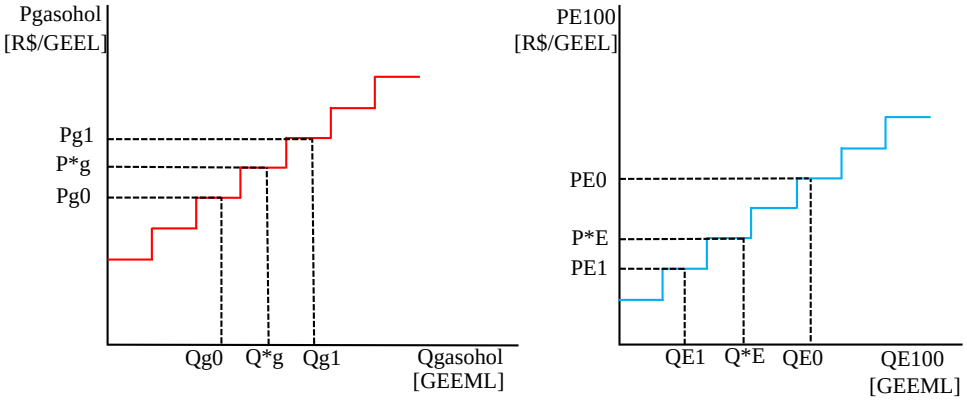

Figure 5.4: Shifts in demand for gasohol and E100[8]

Stochasticity: The model is initialized stochastically. Properties such as farmers' yields, mills' production capacities and drivers' preferences of the relative fuel prices are randomly assigned among the agents. The decision making of farmers agents about expansion of sugarcane fields and the locations of new mills is modeled stochastically based on the probabilities calculated by the PLUC model [189].

Collectives: The model neglects the formation of aggregations among individuals.

Observation: Expansion of the ethanol/sugar production capacity, production of sugar and ethanol, demand of ethanol, and ethanol prices are the main key performance indicators.

[7] Gasoline energy equivalent liters
[8] GEEML: gasoline energy equivalent million liters

Initialization: 418 mill agents, 3715 farmer agents, and 2500 driver agents are initialized for the year 2013. The location of mills and their type (sugar plant, ethanol plant, and flex plant) are based on real spatial data for the year 2013 [199]. The location of the farmers is based on the stochastic projections of the PLUC model for 2013. Table 5.1 presents the parameters that describe the state of the agents at the start of the simulation.

Table 5.1: Parameters used in the initialization of the simulation (representing the year 2013)

Parameter	Value	Brief description	Units
		Farmers	
initial-number-farmers	3715	initial number of farmers	–
farm-a	2500	farm area	ha
yield-SC	75	yield of sugarcane per hectare	$t\,ha^{-1}$
yield-TRS	140	yield of total recoverable sugar per ton of sugarcane	$kg\,t^{-1}$
		Mills	
number-sugar-mill-plants	10	number the sugar plants	–
number-ethanol mill plants	83	number of ethanol plants	–
initial-number-flex-mill-plants	325	number the mills plants	–
proc-capacity[a]	[1, 5]	processing capacity of sugarcane	$Mt\,yr^{-1}$
yield-sugar-SC[b]	U(119, 146)	yield of sugar per ton of sugarcane	$kg\,t^{-1}$
yield-hydrous-SC[b]	U(83, 92)	yield of hydrous ethanol per ton of sugarcane	$l\,t^{-1}$
yield-anhydrous-SC[b]	U(79, 88)	yield of anhydrous ethanol per ton of sugarcane	$l\,t^{-1}$
yield-ethanol-molasses	U(8, 10)	yield of ethanol from molasses per ton of sugarcane	$l\,t^{-1}$
sugar-proc-cost	U(41, 51)	processing cost of sugar per ton of sugarcane	$R\$\,t^{-1}$
hydrous-proc-cost	U(14, 17)	processing cost of hydrous ethanol per ton of sugarcane	$R\$\,t^{-1}$
anhydrous-proc-cost	U(25, 31)	processing cost of anhydrous ethanol per ton of sugarcane	$R\$\,t^{-1}$
prod-ratio-sugar[c]	U(**0.5**, 0.6)	proportion of sugarcane that is used to produce sugar	–
prod-ratio-hydrous[c]	U(0.2,**0.5**)	proportion of sugarcane that is used to produce hydrous ethanol	–
prod-ratio-hydrous-molasses	U(0.2, 0.5)	proportion of ethanol produced from molasses that is used to produce hydrous ethanol	–
		Drivers	
Type		gasohol; flex	–
Demand	47244	energy demand per vehicle	MJ yr
preference-relative-price[c]	N(**0.9**, 0.1)	value in the relative price that determines the consumption pattern of the driver i. Values of the relative price higher than the individual relative price lead to consumption of gasohol by the driver	–
		Global variables	
blend-mandate	23	blend mandate	%
tax-gasoline	1.23	tax levied on gasoline	$R\$\,l^{-1}$
tax-hydrous	0.30	tax levied on hydrous ethanol	$R\$\,l^{-1}$
tax-anhydrous	0.05	tax levied on anhydrous ethanol	$R\$\,l^{-1}$

[a] The distribution of the production capacity was based on Valdes [200].
[b] It is assumed that the differences in the yields are due to differences in industrial efficiencies between mills/distilleries.
[c] The values in **bold** were obtained from the model calibration (see Appendix D).

Input data: The behavior of the model is driven by 7 exogenous parameters: gasoline and sugar prices, number of flex and regular vehicles, productivity of both sugarcane and the TRS content, and sugar demand. The productivity of both sugarcane and the TRS content is assumed to be constant during the period 2013-2030. The values for sugarcane yield and TRS content yield are $75\,t\,ha^{-1}$ and $140\,kg TRS\,t^{-1}$, respectively. These values were set out based on historical developments [201]. Projections for the other parameters up to 2030 were retrieved from the literature (see Table 5.2). The number of vehicles is assumed to be exogenous ought to that they are driven by macro-economic variables such as level of urbanization, population density, and the growth of the Gross

Domestic Product (GDP). Prices can be either current (nominal) prices or constant (real) prices as we assumed an inflation of zero.

Table 5.2: Definition of the exogenous parameters

Year	Sugar demand[a] [Mt]	Nominal sugar price[b] [US$ kg^{-1}]	Nominal crude oil price[c] [US$ bbl^{-1}]	Number Flex Vehicles[d] [millions]	Number Regular Vehicles[d,e] [millions]
2013	34.85	0.39	104.08	23	15
2014	35.92	0.37	96.2	26	14
2015	36.94	0.3	50.8	28	13
2016	37.88	0.4	42.8	30	13
2017	38.76	0.4	55	32	13
2018	39.58	0.4	60	35	13
2019	40.33	0.4	61.5	37	13
2020	41.01	0.4	62.9	40	13
2021	41.63	0.39	64.5	43	13
2022	42.19	0.39	66	46	13
2023	42.67	0.39	67.6	49	14
2024	43.09	0.39	69.3	53	14
2025	43.45	0.39	71	56	14
2026	43.74	0.39	72.8	59	14
2027	43.97	0.39	74.6	62	15
2028	44.13	0.38	76.4	66	16
2029	44.22	0.38	78.2	69	17
2030	44.25	0.38	80	73	17

[a] The demand of sugar was calculated based on results reported by the MAGNET model [19].
[b] Retrieved from [202]. The ratio of domestic price of sugar to the international price is 1:1.2 [203].
[c] The ratio of crude oil price to gasoline price is 1:1.2 [204].
[d] Retrieved from [205, 206].
[e] Regular vehicles only can use gasohol (blend of gasoline and anhydrous ethanol. The maximum blend of anhydrous ethanol in gasohol is 27.5% v/v).

Submodels: The algorithm that describes the investment in new processing capacity consists of four steps. This algorithm is followed by every single mill owner. The first step is to assess the financial status. It is assumed that mill owners are willing to invest in new processing capacity if they are making profits. The second step is to forecast the demand of sugar and ethanol. If this demand is increasing, then mill owners determine the profitability of building a new processing capacity by calculating the net present value (NPV) of the project. Finally, if the project is profitable (i.e. $NPV > 0$), then mill owners invest in new processing capacity. The values of the parameters used in the net present value calculation are reported in Table 5.3-Table 5.5. It is assumed that mill owners have a different perception of risk in the investment. This difference in the perception of the risk was captured by using different values for the discount rate.

Critical assumptions that underpin the model structure are:

- Brazilian policies are constant during the modeled timeframe.

Table 5.3: Estimates of fixed capital investment costs and processing costs [9]

Capacity	Sugar		Ethanol	
[Mt yr^{-1}]	Fixed Capital Investment[a] [MUS$]	Processing cost[b] [MUS$ yr^{-1}]	Fixed Capital Investment[a] [MUS$]	Processing cost[c] [MUS$ yr^{-1}]
1	32.05	8.84	32.13	8.88
3	69.16	26.52	101.83	26.64
5	98.89	44.19	173.02	44.44

[a] Based on the data reported in [207].
[b] Based on the data reported in [208].
[c] Based on the data reported in [209].

Table 5.4: Financing and production assumptions

Parameter	Value	Unit
plant lifetime	20	yr
installation time	3	yr
Income tax rate[a]	37	%
depreciation period	10	yr
discount rate[b]	U(10,20)	%

[a] Reference value for Brazil.
[b] Flex owners of flex plants differ in their perception of risk in the investment decision. Here, we use the discount rate as proxy for risk perception. The difference in risk perception among owners of flex plants was modeled by using a uniform distribution.

Table 5.5: Plant start-up schedule

Year	TCI schedule	Plant availability (% of capacity)
-2	33,33% Fixed Capital	0
-1	33,33% Fixed Capital	0
0	33,33% Fixed Capital	0
1		30
2		70
3		100

- Brazil is an open system. That is, Brazil can either import or export ethanol if required.
- There are neither import tariffs nor export tariffs for ethanol.
- The international price of ethanol is endogenous and it is calculated based on the

[9] Include all the processing costs other than the feedstock cost.

domestic price. The ratio of domestic price of ethanol (both hydrous and anhydrous) to the international price of ethanol is 1:1.3 [210].

- The exchange rate of Brazilian reais to US dollars is constant during the timeframe.
- The international demand for hydrous and anhydrous ethanol is a sink. This demand is considered only when the domestic demand for ethanol is already satisfied. Imports of ethanol are only considered if there is a shortage in the domestic production.
- The fuel preferences of drivers remain constant during the timeframe of the simulation.
- The share of electric vehicles in the road transport sector is negligible during the timeframe of the simulation.
- Economic resources are available for new investments in processing capacity of sugarcane.

5.2.3. MODELING THE BIOFUEL POLICIES

The blend mandate and the taxes levied on gasoline and ethanol shape the behavior of the ethanol market by influencing the ethanol prices and the mandate for anhydrous ethanol. Ethanol prices along with gasoline and sugar prices influence actors' decision making on production, consumption, and investment. The price of gasohol hinges on the gasoline price, anhydrous ethanol price, gasoline tax, anhydrous tax, and blend mandate. Similarly, the price of E100 hinges on the hydrous ethanol price and the tax levied on hydrous ethanol. The total supply of gasohol in the market is based on the total production of anhydrous and the blend mandate. The total supply of E100 into the market is equivalent to the total production of hydrous ethanol. Taxes and blend mandates are assumed to be constant during the time frame of the simulation. The mapping between biofuel policies and prices and demand is presented below [171, 187]:

$$P_F = \alpha(P_A + t_A) + (1-\alpha)(P_G + t_G) \tag{5.11}$$

$$P_{E100} = P_H + t_H \tag{5.12}$$

$$\alpha = \frac{V_A}{V_F} \tag{5.13}$$

Where P_F, P_A, P_G, P_{E100}, and P_H are the price of gasohol, anhydrous ethanol, gasoline, E100, and hydrous ethanol, respectively in Reais per liter. t_A, t_G, and t_H are the taxes levied on anhydrous ethanol, gasoline, and hydrous ethanol, respectively in Reais per liter. α denotes a blend mandate for anhydrous ethanol. V_A and V_F are the volumes of anhydrous ethanol and gasohol, respectively in liters.

The structure of the fuel taxes in Brazil is complex. Taxes vary by state and they may be changed at any point in time. To cope with this complexity, we assumed that taxes remain constant during the timeframe of the simulation. We also assumed homogeneity

in the distribution of fuel taxes in Brazil. That is, fuel taxes are equally enacted in the different states of Brazil. In this study, we use as a baseline the values reported by de Gorter et al. [171] for the period 2011/2012 in the state of Sao Paulo. Based on this baseline scenario, we defined extreme scenarios for the fuel taxes. One extreme consists of fuel taxes equivalent to the double of those reported in the baseline. The other extreme consists of tax free fuels. The blend mandate scenarios were defined based on the baseline, the minimum requirement of blending, and the blending wall. Table 5.6 presents the values used in the baseline and extreme scenarios.

Table 5.6: Values used for the policy instruments in the baseline and extreme scenarios

Policy instrument	Scenario			
	Low	Baseline	High	Units
Gasoline tax	0	1.23	2.46	$R\$l^{-1}$
Hydrous ethanol tax	0	0.3	0.6	$R\$l^{-1}$
Anhydrous ethanol tax	0	0.05	0.1	$R\$l^{-1}$
Blend mandate	20	23	26	%

5.3. RESULTS

IN this section, we describe the results of the influence of three different levels of blend mandate and tax levied on hydrous ethanol and gasoline on the development of the sugarcane-ethanol market. We focus on four relevant aspects: the expansion of sugarcane processing capacity, the location of new processing facilities, consumption patterns of flex vehicle owners, and production of sugar, hydrous and anhydrous ethanol.

The results are presented in a matrix of 9 panels defined by the blend mandate and the gasoline tax variables. The effect of the hydrous tax is presented by different colors in each panel. For a given tax levied on anhydrous ethanol, the 9 panels describe all of the possible permutations among blend mandate and taxes levied on gasoline and hydrous ethanol (see Table 5.6). The results presented below correspond to a tax levied on anhydrous of 0.05 $R\$l^{-1}$ as the effect of the anhydrous tax on investment in processing capacity, production and consumption of ethanol is negligible (see Appendix E).

5.3.1. SPATIAL PATTERN AND EVOLUTION OF SUGARCANE PROCESSING CAPACITY.

Figure 5.5 and Figure 5.6 show the evolution of the processing capacity for different combinations of gasoline tax, blend mandates, and tax levied on hydrous ethanol. As expected, the investment in new processing capacity of sugarcane increased as the gasoline tax increase. In the period 2020-2030, with a hydrous tax of 0.3 $R\$l^{-1}$, the investment in new processing capacity grows at the average rate of 0.38% (see Figure 5.5.a) and 6.61% (see Figure 5.5.c) per year. The investment in new processing capacity increased as the blend mandate increased only when the tax levied on gasoline was 0 $R\$l^{-1}$ and 1.23 $R\$l^{-1}$, respectively. In the period 2020-2030, with a tax levied on hydrous ethanol of 0.6 $R\$l^{-1}$, the investment in new processing capacity grows at the average rate of 0.45%

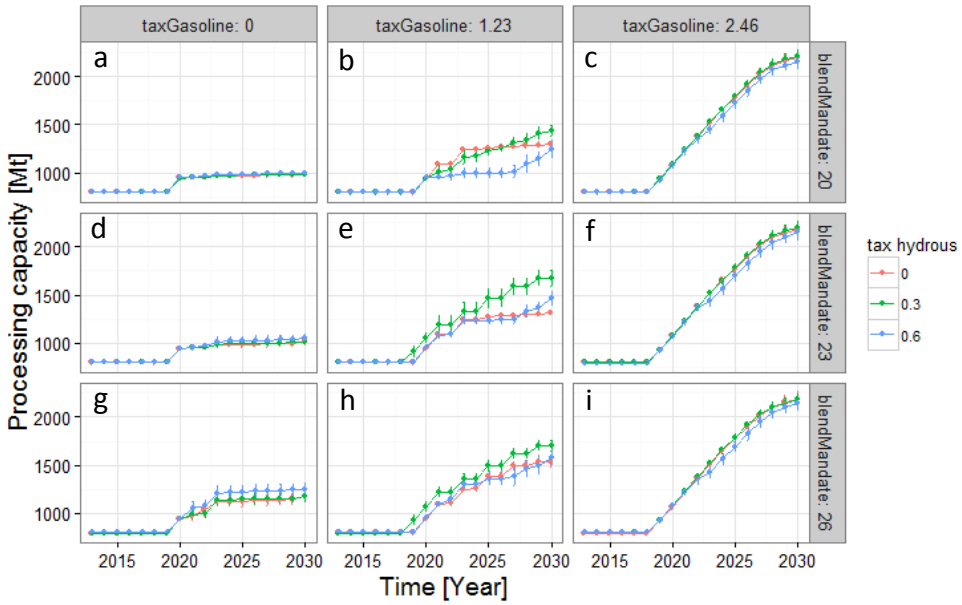

Figure 5.5: Sugarcane processing capacity as a function of time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.05 R$l^{-1}. Forty repetitions were carried out in the simulations for each combination of policy instruments. Dots and the err bars represent the mean and the standard deviation over these forty repetitions, respectively.

(see Figure 5.5.a) and 2.53% (see Figure 5.5.g) per year. With a gasoline tax of 2.46 R$l^{-1}, the effect of the blend mandate on the investment of processing capacity of sugarcane was negligible.

The hydrous tax only caused difference between scenarios in the investment of new processing capacity of sugarcane when the gasoline tax was 1.23 R$l^{-1}. The investment in new processing capacity was higher when the hydrous tax was 0.3 R$l^{-1}. In the period 2020-2030, when the taxes levied on hydrous ethanol are 0 R$l^{-1}, 0.3 R$l^{-1}, and 0.6 R$l^{-1}, the investment in new processing capacity grows at the average rate of 2.94%, 3.89%, and 2.43% per year, respectively (see Figure 5.5.b). This behavior is because in this regime both prices of hydrous and anhydrous ethanol influence the decision making on investment in new processing capacity. When there is a tax exemption for hydrous ethanol, the demand for hydrous ethanol increases, which leads to an increase in the price of hydrous ethanol and to a decrease in the price of anhydrous ethanol. Nevertheless, the increase in hydrous price is insufficient to offset the effect of low anhydrous price on the investment decision. A similar mechanism is activated when the tax levied on hydrous ethanol is 0.6 R$l^{-1}. In this case, the increase in anhydrous ethanol price is insufficient to offset the effect of low hydrous price on the investment decision. Therefore, the investment in total sugarcane processing capacity when the hydrous tax is 0 R$l^{-1} and 0.6 R$l^{-1} is less than that invested when the hydrous tax is 0.3 R$l^{-1}. The effect of the tax levied on anhydrous ethanol on the expansion of the processing capacity

was negligible (see Appendix E).

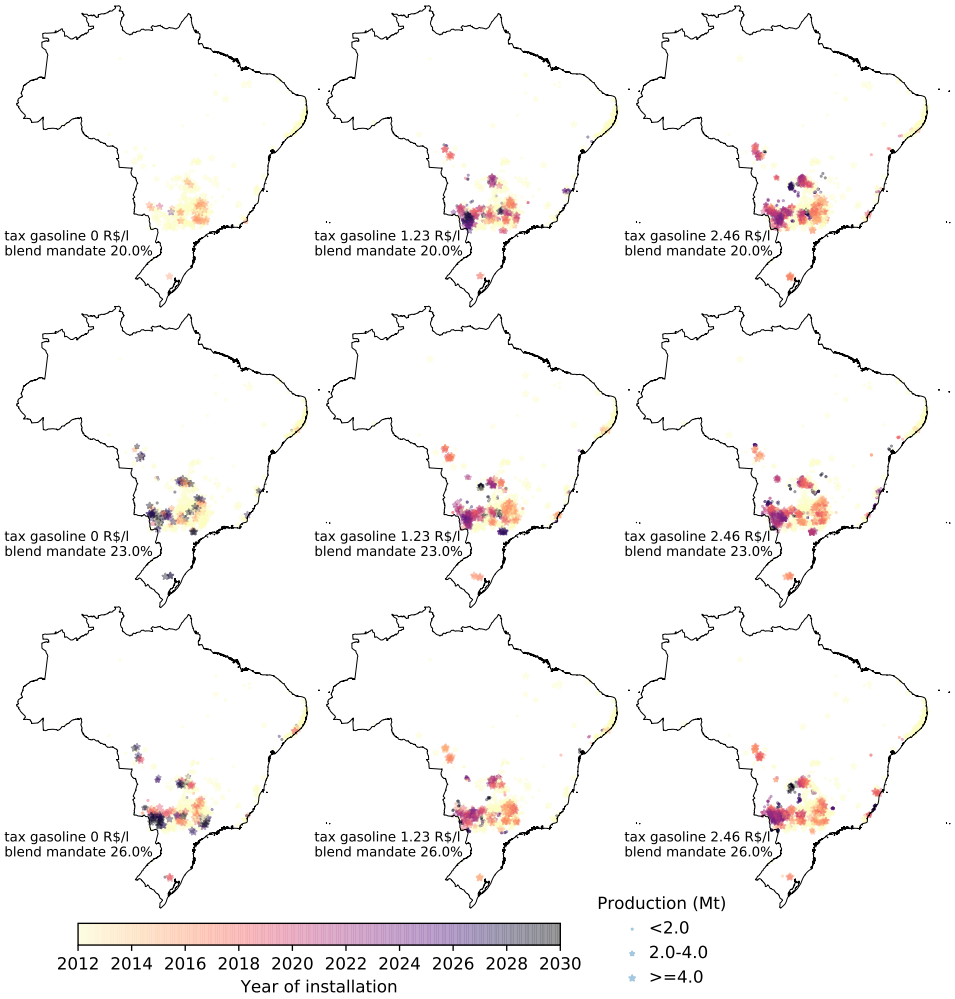

Figure 5.6: Location, year of installation, and processing capacity of sugarcane plants as a function of different combinations of blend mandate and gasoline tax. Tax on gasoline in $R\$l^{-1}$. Blend mandate in %v/v. Hydrous tax = 0.3 $R\$l^{-1}$. Anhydrous tax = 0.05 $R\$l^{-1}$. This figure shows the results for a single simulation run. To show that the patterns shown here are representative across runs with the same policy instrument values, results for another simulation run out of the forty repetitions are presented in Appendix E.

The spatial pattern (Figure 5.6) shows that the expansion started in the center of Sao Paulo state, moved to Goiás and a small part of Mato Grosso, and finalized in the west side of Mato Grosso do Sul state. The majority of processing capacity of these plants was approximately 5 Mt. An increase in the gasoline tax led to a continuous deployment of

new plants across the timeframe, resulting in a more pronounced east-west expansion pattern.

5.3.2. CONSUMPTION PATTERNS OF FLEX VEHICLES

The percentage of owners of vehicles (flex and gasohol) demanding E100 (hydrous ethanol) was influenced by the interaction between the gasoline tax and hydrous tax (Figure 5.7). In 2030, the mean percentage of consumers of E100 increases 20% when the gasoline tax increases from 1.23 R$l^{-1} to 2.46 R$l^{-1} and there is a tax exemption on hydrous ethanol. For hydrous taxes of 0, 0.3, and 0.6 R$l^{-1}, the mean percentage of consumers of E100 in 2020 is 60%, 41%, and 29%, respectively (see Figure 5.7.f). In general, an increase in the gasoline tax and a reduction in the hydrous tax led to an increase in the consumption of hydrous ethanol. As expected, a tax exemption on gasoline led to very low consumption of ethanol.

At values of gasoline tax of 1.23 and 2.46 R$l^{-1}, the development of crude oil prices influenced the behavior of the consumption patterns of flex vehicles users (see Table 5.2, column 4). This pattern is characterized by a dip in the consumption of E100 in 2017. The consumption patterns of owner of flex vehicle were independent of the level of blend mandate. The effect of the tax levied on anhydrous on the share of flex vehicle users consuming E100 was also negligible (see Appendix E).

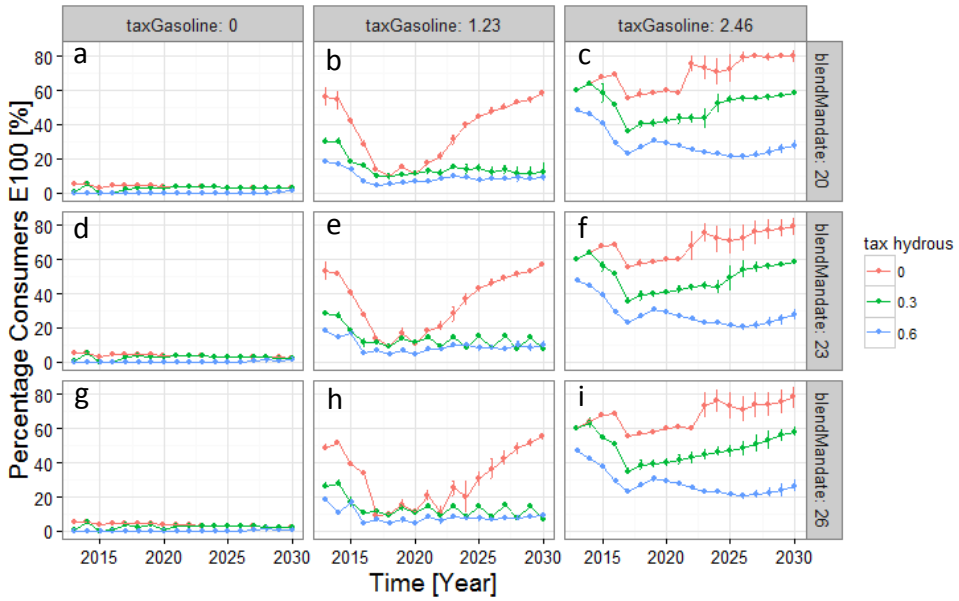

Figure 5.7: Percentage of flex vehicle owners that consume E100 over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.05 R$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments

5.3.3. PRODUCTION OF SUGAR, HYDROUS AND ANHYDROUS ETHANOL.

Patterns in the production of sugar are connected to patterns in the expansion of processing capacity (see Figure 5.5 and Figure 5.8). This connection hinges on the gasoline tax. A tax free gasoline regime favors the production of sugar compared to ethanol. The production of sugar, however, is limited by the rate of expansion of processing capacity. On the contrary, in a regime characterized by a high gasoline tax, the production of sugar is driven by the rate of expansion of processing capacity as this regime favors the production of ethanol. The effect of the blend mandate, tax levied on hydrous ethanol and anhydrous ethanol (see Appendix E) on sugar production is negligible.

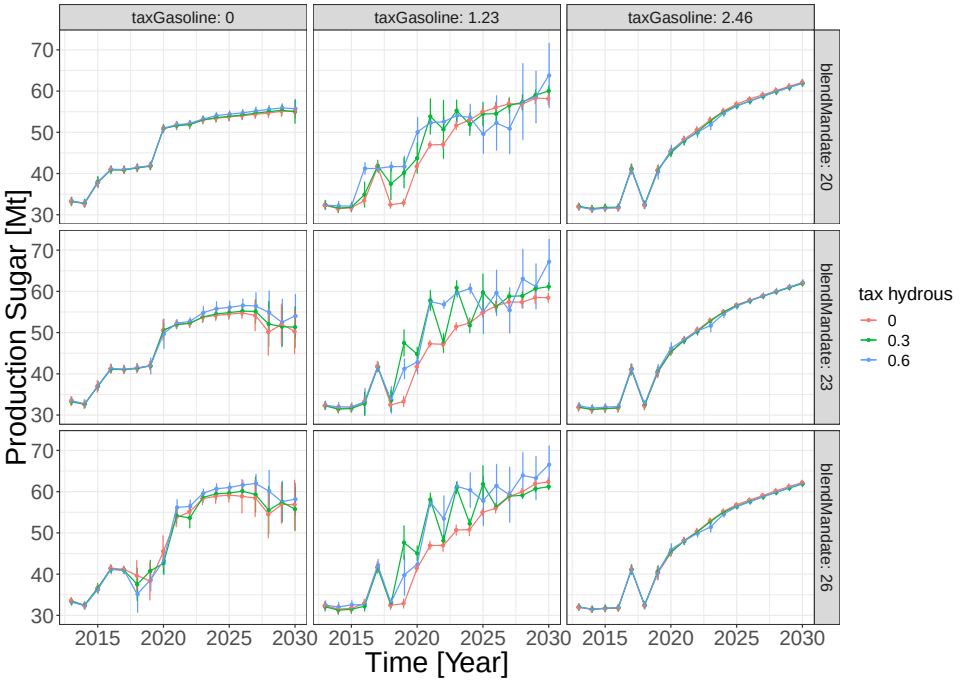

Figure 5.8: Total production of sugar in Brazil over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R\$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.05 R\$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

As shown in Figure 5.9, an increase in the gasoline tax led to an increase in the production of hydrous ethanol and to a decrease in the production of anhydrous ethanol. Furthermore, an increase in the tax levied on hydrous ethanol led to a decrease in the production of hydrous ethanol and to an increase in the production of anhydrous ethanol. When there was a tax exemption for gasoline, the effect of the hydrous tax on the production of both hydrous and anhydrous ethanol was negligible.

For values in the blend mandate of 23% and 26%, a gasoline tax of 1.23 R\$l^{-1}, hydrous tax of 0.3 R\$l^{-1}, and anhydrous tax of 0.05 R\$l^{-1}, an oscillating behavior was observed in the production of hydrous and anhydrous ethanol. This behavior is due to the interplay

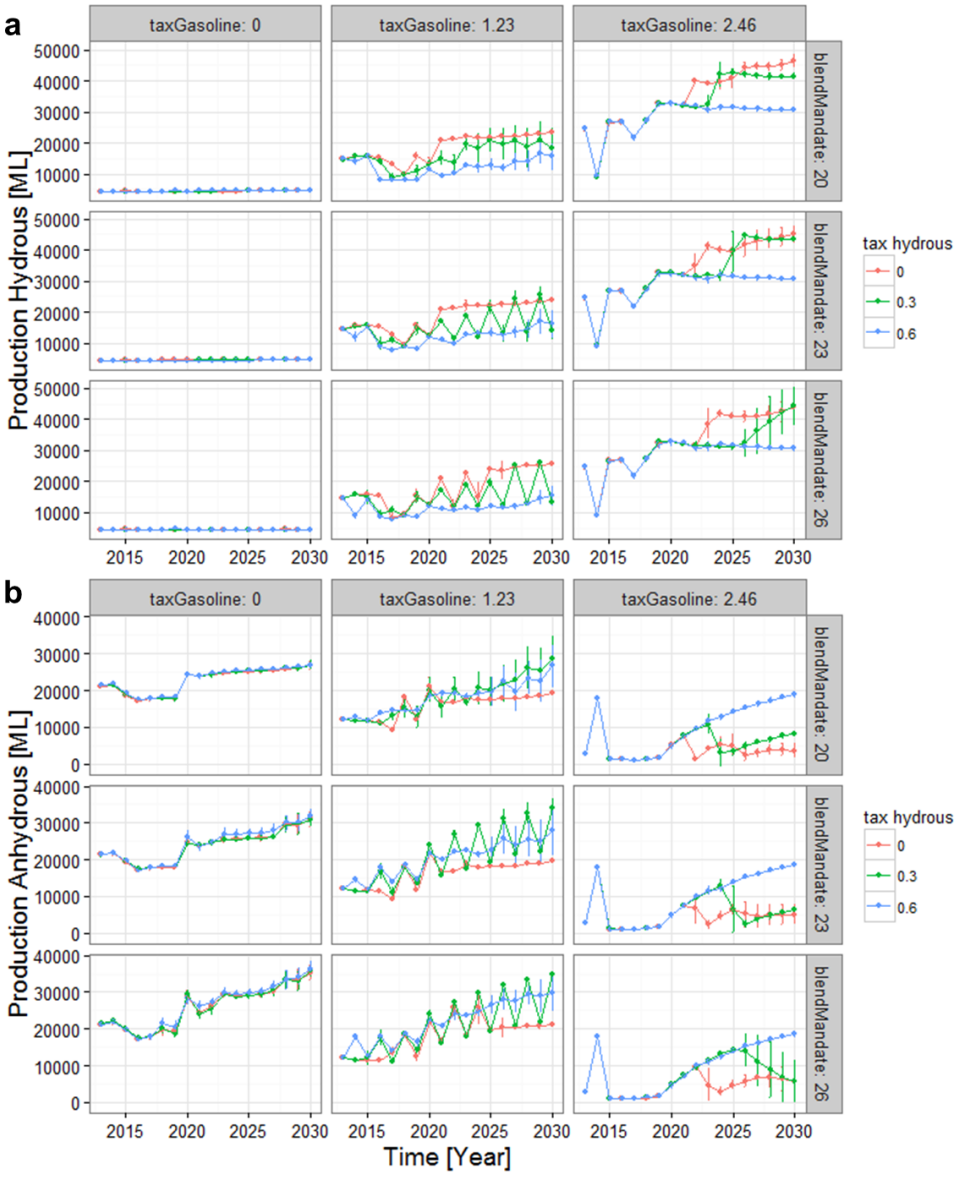

Figure 5.9: Total production of hydrous **(a)** and anhydrous ethanol **(b)** in Brazil over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R\$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.05 R\$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

of two factors. First, the fuel choice of owners of flex vehicles shifts between two states when the tax levied on hydrous ethanol is 0.3 R$l^{-1}. The second factor is the myopic behavior of the owners of the mills plants as to production of ethanol. In economic theory, this oscillating behavior in the production of ethanol is described by the Cobweb theory [211].

The dip in the production of hydrous ethanol in 2014, when the gasoline tax was 2.46 R$l^{-1}, is due to two factors: the myopic behavior of owners of flex plants and the extreme options as to the production of hydrous and anhydrous ethanol. At this level of the gasoline tax, flex plants are incentivized to produce only hydrous ethanol unless the price of anhydrous ethanol is high enough, in that case, flex plants drastically reduce the production of hydrous ethanol. This situation happened in 2013, when the crude oil price was high, which led mill owners to reduce the production of hydrous ethanol in 2014 because of their myopic behavior.

For a gasoline tax of 1.23 R$l^{-1} and a hydrous tax of 0.3 R$l^{-1}, an increase in the blend mandate magnified the oscillating behavior in the production of both hydrous and anhydrous ethanol. For the rest of permutations between gasoline tax and hydrous tax, the effect of the blend mandate on the production of hydrous and anhydrous was negligible. As shown in Appendix E, the effect of the anhydrous ethanol tax on the production of hydrous and anhydrous ethanol was also negligible.

5.4. DISCUSSION

WE found that under the set of chosen policy measures, the expansion of the sugarcane processing capacity in Brazil is driven most by a high gasoline tax (see Figure 5.5), provided that the policy landscape remains stable, that the effect of import and export tariffs on the market is negligible, and that the share of electric vehicles in the road transport sector remains small up to 2030. This insight is in line with that reported by Demczuk & Padula [34].

An increase of the gasoline tax leads to a continuous deployment of new plants between 2015 and 2030. The pattern of expansion shows an east to west pattern, from Sao Paulo state to Goiás, Mato Grosso, and Mato Grosso do Sul (see Figure 5.6). These patterns are in line with those reported by Lapola *et al.*[186], for it is expected that the deployment of new processing capacity will take place predominantly on productive lands. Also, a general trend was found in the deployment of new processing capacity. This trend is characterized by the deployment of large scale sugarcane processing capacity plants. This finding is in line with the results reported by Jonker *et al.* [19].

We found that the consumption pattern of the owners of flex vehicles hinges on the interaction among gasoline prices and taxes levied on gasoline (see Figure 5.7). Namely, the gasoline tax exhibits a correlated effect on E100 demand. This finding is in line with those of de Freitas & Kaneko [179]. Finally, we found that the production patterns of sugar, hydrous and anhydrous ethanol are influenced by the gasoline tax (see Figure 5.8 and Figure 5.9). A tax-free regime favours the production of sugar compared to ethanol but limits the increase in its production over time. An increase in the gasoline tax leads to an increase in the production of hydrous ethanol and to a decrease in the production of anhydrous ethanol.

For the Brazilian government that strives for enhanced consumption of renewable

fuels in the energy mix, our findings suggest that an increase in the gasoline tax (above 1.23 Rl^{-1}) and a reduction in the hydrous tax (less than 0.3 Rl^{-1}) may lead to doubling the production of ethanol by 2030 (relative to 2016). Nevertheless, the government needs to be cautious when implementing this policy as it can have negative impacts on the productivity level of ethanol producers or in the ethanol prices. The gasoline tax may disincentive ethanol producers in striving for technological improvements as this protection mechanism guarantee that ethanol is competitive with gasoline. One subject that remains to be explored is to what extent the gasoline tax should be increased to incentivize the investment in processing capacity.

5.5. CONCLUSIONS

THis study was conducted to answer the following research question: *what is the combined effect of a blend mandate and a tax levied on gasoline, hydrous, and anhydrous ethanol on the development of the ethanol market in Brazil?* To answer this question, we developed an agent-based model of the Brazilian ethanol market.

We found that the evolution of the Brazilian ethanol market is driven mostly by a gasoline tax. A high gasoline tax leads to increased investment in sugarcane processing capacity, to an increase in the consumption of E100, and to an increase in the production of hydrous ethanol. Given that the Brazilian government aims to increase the consumption of hydrous ethanol in the energy mix in 2030, and thus needs to double the supply of ethanol, our findings suggest that this goal is achievable if the gasoline tax is increased above 1.23 Rl^{-1} and the hydrous ethanol is tax-free.

Our study applies a number of key enhancements to prior studies. First, it models the expansion of the sugarcane processing capacity in Brazil spatially-explicit, as the investment decision making in new sugarcane processing capacity is bound to the land availability and location [212]. Second, it incorporates the CONSECANA-SP mechanism to model the interaction between farmers and producers. Finally, it includes preferences in and variation between the decision making of consumers. Overall, these characteristics have been neglected in previous analyses to ensure mathematical tractability and rigor. As we show here, agent-based modelling allows a richer description of the system without sacrificing the desirable rigor of formal analysis.

This approach, however, does have some limitations. First, the current instability of the policy landscape in Brazil is neglected. The policy instruments are subject to change in shorter time frames. For instance, in reality, the blend mandate is adjusted depending on the industry capacity to deliver ethanol, oil prices, and size of the fleet. This instability might increase the perceived risk level in decisions on whether or not to invest in processing capacity. Second, technological innovations in the road transport sector have been neglected. The introduction of e.g., electric vehicles, can drastically change fuel consumption patterns. Third, the effect of import and export tariffs on the Brazilian ethanol market is neglected. Fourth, we neglected the role of distribution companies and gas stations owners on the final prices of ethanol.

Moreover, the heuristics used to model the decision making as to the production of hydrous and anhydrous ethanol under extreme values of the gasoline tax (0 Rl^{-1} and 2.46 Rl^{-1}) need to be improved. Further research should map the relationship between gasoline tax and decision making as to ethanol production. Given the important role

that distribution companies and gas station owners play on the determination of ethanol prices, we also recommend to investigate the effect of the market power of distribution companies and gas stations owners on the evolution of the Brazilian sugarcane-ethanol supply chain, and what factors play an important role in the emergence of these cartels. We also recommend assessing the impacts of the variation of taxes and mandates by state on the evolution of the system, as favorable tax regimes may incentivize the production of ethanol in expansion areas. Finally, inasmuch as the Brazilian policy landscape is leaning to spur the production of advanced biofuels (2^{nd} generation biofuels), we recommend researching the emergence of 2^{nd} generation ethanol supply chains and their co-evolution with sugarcane-ethanol supply chains in the Brazilian context.

Yet, this study provides new insights into the workings of the Brazilian ethanol market under different policy landscapes. A further step would be the institutional design of the Brazilian ethanol market. The approach proposed in this study could be used to guide the institutional design process. Namely, the agent-based model could be used to assess the impact of different, potentially new, policy instruments on the ethanol market. Specifically, policy instruments aimed to increase both investments in sugarcane processing capacity and hydrous ethanol production.

All in all, as biomass/biofuel markets are complex and context-dependent, we argue that we should strive for developing models that incorporate the necessary mechanisms for a reliable description of the problem at hand, instead of using only one modeling paradigm (i.e. Computational General/Partial Equilibrium Models) to analyze different problems in different geographies. This study is a step forward in the development of an ecology of models that provides a richer description of biomass/biofuels markets. The agent-based model developed in this study illustrates how to incorporate the effect of preferences into the actors' decision making, how to include governance structures, and how to map biofuel policies onto actor behavior. As we show here, these elements and their interaction are necessary to produce system behavior. Notwithstanding their importance, these elements are neglected by mainstream approaches.

6

EXPLORING THE EMERGENCE OF A BIOJET FUEL SUPPLY CHAIN IN BRAZIL

If you didn't grow it,
you didn't explain its emergence.

Josh Epstein *(1999)*

The world is complex,
and we capture it with different languages,
each appropriate to the process which we are describing.
Every complex process can be addressed and understood in
different languages and at different levels.

Carlo Rovelli, *Seven brief lessons on physics*

This chapter has been submitted to a scientific journal

The aviation industry accounts for more than 2% of global CO_2 emissions. Biojet fuel is expected to make an essential contribution to the decarbonisation of the aviation sector. Brazil is seen as a key player in developing sustainable aviation biofuels owing to its long standing experience with biofuels. Nevertheless, a clear understanding of what policies may be conducive to the emergence of a biojet fuel supply chain is lacking. We extended a spatially-explicit agent-based model to explore the emergence of a biojet fuel supply chain from the existing sugarcane-ethanol supply chain. The model accounts for new policies (feed-in tariff and capital investment subsidy) and new considerations into the decision making about production and investment in processing capacity. We found that in a tax-free gasoline regime, a feed-in tariff above $3\,\mathrm{R\$l^{-1}}$ *stimulates the production of biojet fuel. At higher levels of gasoline taxation (i.e.* $2.46\,\mathrm{R\$l^{-1}}$*), however, any feed-in tariff is insufficient to ensure the production of biojet fuel. Given the current debate about the future direction of the biofuel policy in Brazil, we recommend further research into the effect of market mechanisms based on greenhouse gas emissions on the emergence of a Brazilian biojet fuel supply chain.*

6.1. INTRODUCTION

THE aviation industry accounts for more than 2% of global CO_2 emissions [15]. To reduce the environmental impact of the aviation sector, the Air Transport Action Group (ATAG) has established goals to reach carbon neutral growth from 2020 and reduce net carbon dioxide emissions by 50% (relative to 2005 levels) by 2050 [16]. Unlike for the road transport sector, short-term options to decarbonize the air transport sector are limited. Aviation will rely on liquid fuels with high energy density for decades to come [16]. Biojet fuel is expected to make an essential contribution to the decarbonisation of the aviation sector [17]. Nevertheless, production volumes of biojet fuel have been negligible as demand remains low because of high prices [213]. The lack of competitiveness of biojet fuel as compared with jet kerosene is one of the main factors hindering the emergence of biojet fuel supply chains.

Brazil is seen as a key player in developing sustainable aviation biofuels owing to its long standing experience with biofuels and its increasing demand for jet fuel [214]. Currently, Brazil consumes 6 Mton/year of jet fuels and it is projected that the required jet fuel amounts to over 20 Mton/year in 2050 [215].The research into the potential of up taking RJF production in Brazil has mainly focused on availability of feedstocks [216], techno-economic and environmental impact assessments [217, 218]. Although the Brazilian ethanol and biodiesel supply chains are a clear example of the benefits of long-term policies on the development of the bioenergy sector [177], not much attention has been hitherto paid to the influence of policies on the emergence of biojet fuel supply chains

6.1.1. LITERATURE REVIEW

A recent strand of literature has focused on the effect of policy instruments on the aviation sector's economic and environmental performance. The most studied policy instruments include the EU emission trading scheme (ETS) [219–221], the US federal aviation administration [222], and carbon pricing [223].

In the analysis of the implications of including the aviation sector in the European emission trading scheme (EU-ETS), Anger found that this policy has a negligible effect on the EU economy, and leads to reductions in the CO_2 emissions [219], whereas Vespermann and Wald concluded that the air transport sector is unable to yield significant reductions of emissions under the EU-ETS [220]. Scheelhaase *et al.* found that including the aviation into the ETS would incentive airports to maximize their output in terms of RTK[1] in 2010 regardless of the emissions caused, and would have a moderate impact on prices increases [221].

To assess the impacts of the US Federal Aviation Administration (FAA) on the economic and environmental performance, Winchester *et al.* used an economy-wide model coupled with a partial equilibrium model of the aviation industry. The authors found that meeting the aviation biofuel target has a small impact on CO_2 emissions and that it is an expensive abatement option relative to alternatives [222].

Sgouridis *et al.* developed the Global Aviation Industry Dynamics (GAID) model to assess the impact of five generic policies (i.e. (i) technological efficiency improvements, (ii) operational efficiency improvements, (iii) use of alternative fuels, (iv) demand shift,

[1] Revenue tonne kilometers.

and (v) carbon pricing) on the reduction of emissions of the aviation sector. The authors found that improvements in the efficiency of technology, use of biofuels, moderate levels of carbon pricing, and reduction in short and medium haul travel are required for the transition of the aviation sector to sustainable mobility [223].

De Jong used a cost optimization model (RESolve-Biomass) to project the consumption of renewable jet fuel (RJF) in the EU and its environmental performance. The model accounts for the anticipated regulatory context in the EU (i.e. RED-I, RED-II proposal[2], the EU Emission Trading scheme (EU ETS), and the Global Offsetting and Reduction Scheme for International Aviation (CORSIA)), competition for biomass from other bio-based sectors, and the availability of biomass and conversion technologies. He found that a 1.2 multiplier for RJF, (advanced) biofuel targets, and high prices of fossil jet fuel relative to other fossil fuels drive the introduction of RJF in the EU. Nevertheless, a higher multiplier may lead to lower GHG emission reductions [224].

These studies have focused on understanding the impact of certain policies on the aviation sector. As they used models that either assume the existence of static equilibria or assume that the dynamics of the system is governed by the predetermined system structure, none of these studies explored the institutional conditions for the emergence of a biojet fuel supply chain.

The contribution of this work is to provide insights into the institutional conditions that might lead to the emergence of a biojet fuel supply chain from the existing Brazilian sugarcane-ethanol supply chain. The analysis focuses on the impact of institutions on actors' decision making about production and consumption of biofuels. Thus, the spatially-explicit agent-based model that describes the Brazilian sugarcane-ethanol supply chain (see Moncada *et al.* [225]) was extended to account for the processes and mechanisms that may lead to the emergence of a biojet fuel supply chain. The aim of the model is to answer the following research question: *Under what institutional conditions (i.e. formal policies) may the biojet fuel supply chain emerge in Brazil in the period 2015-2030?*

The remainder of the chapter is organized as follows. Section 6.2 describes the conceptual framework that underpins the development of the agent-based model. Section 6.3 describes the results obtained which are discussed in Section 6.4. Finally, conclusions are presented in Section 6.5.

6.2. THEORY AND METHODS

THIS section describes the concepts and modeling considerations required for the potential emergence of a biojet fuel supply chain. We divided this section in four subsections. In the first subsection, we give a brief description of the Brazilian sugarcane-ethanol supply chain and argue why this supply chain can be used as a starting point for the emergence of a biojet fuel supply chain. Then, we describe how the biojet fuel supply chain is conceptualized. In the third subsection, we describe the agent-based model using the ODD protocol[3]. Finally, we describe how we modeled the policies that aim to

[2] The RED-II proposes a multiplier to incentivize the production of biofuels for the aviation and marine sectors. Renewable fuels supplied to these sectors may count 1.2 times their energy contents towards the target.

[3] The Overview, Design concepts, and Details (ODD) protocol is a method used to describe agent-based models. This protocol was developed by Grimm *et al.* [195]

incentivize the investment in and production of biojet fuel.

6.2.1. SYSTEM DESCRIPTION

In this study, we use the Brazilian sugarcane-ethanol supply chain as a "seed" to "grow" a biojet fuel supply chain. The main actors in the sugarcane-ethanol supply chain are farmers, mills owners, fuel suppliers, and drivers. This supply chain has been shaped by governmental support (e.g. ProAlcool program) and the introduction of technological innovations such as flex plants and flex vehicles. Flex technology enables plants to produce flexible ratios of sugar and ethanol from sugarcane [175]. With regard to ethanol, the plants can produce either hydrous ethanol (up to 4.9% v/v of water), or anhydrous ethanol (up to 0.4% v/v of water), or both. Similarly, the introduction of flex vehicles brought flexibility into the demand side of the supply chain. This demand consists of mostly flex vehicles and regular vehicles. Flex vehicles can be powered by a mix of E100 (hydrous ethanol) and gasohol (a blend of gasoline and anhydrous ethanol, of which the max share of anhydrous ethanol is 27.5% v/v due to technical limitations of regular vehicles [34]) in any ratio. Unlike flex vehicles, regular vehicles can be only powered by gasohol.

Institutional arrangements and policy instruments influence the behavior of the ethanol supply chain. One of the most important institutional arrangements is CONSECANA-SP. This institutional arrangement reduces the uncertainty in the interaction between farmers and mill owners by determining the price of sugarcane. This price is determined by the amount of total recoverable sugar (TRS) in the sugarcane and the prices of sugar and ethanol on the domestic and foreign markets [180]. On the other hand, policy instruments such as blending mandates (e.g. of anhydrous ethanol in gasohol) and taxes levied on hydrous ethanol, anhydrous ethanol, and gasoline influence the behavior of the supply chain by shaping the patterns of production and consumption of ethanol.

One of the main factors hindering the production of biojet fuel is its lack of economic competiveness as compared to fossil jet fuel [213]. The gap between the fossil jet fuel price and the biojet fuel price could be reduced by using existing social and physical infrastructure. In this study, we use the social and physical infrastructure defining the sugarcane-ethanol supply chain to breed a biojet fuel supply for two main reasons. First, the existence of a well-established agro-industrial sector dedicated to the production of ethanol [226]. Second, biojet fuel can be produced from ethanol through the route alcohol to jet fuel. This route involves four steps (see Figure 6.1): dehydration of ethanol, oligomerization of ethylene, distillation of wide spectrum hydrocarbon, and hydrogenation of the saturated hydrocarbon. Recently, ASTM approved a biojet fuel produced from isobutanol for commercial use in blends of a maximum level of 30% in kerosene [227]. About 0.1 $t_{CO_2}\,m^{-3}$ is saved when diverting the displacement of gasoline to the displacement of kerosene[4].

The emergence of a biojet fuel supply chain in the Brazilian context requires the addition of new elements into the existing sugarcane-ethanol supply such as actors (i.e. airports), technology (alcohol to jet fuel) and institutions supporting the introduction

[4]The benefit in terms of carbon balance of diverting the displacement of gasoline to the displacement of kerosene was calculated based on an energy content of 34 561 $MJ\,m^{-3}$ and 34 693 $MJ\,m^{-3}$ and an Carbon Dioxide equivalent of 85 $g_{CO_2e}\,MJ^{-1}$ and 87.5 $g_{CO_2e}\,MJ^{-1}$ for gasoline and kerosene, respectively.

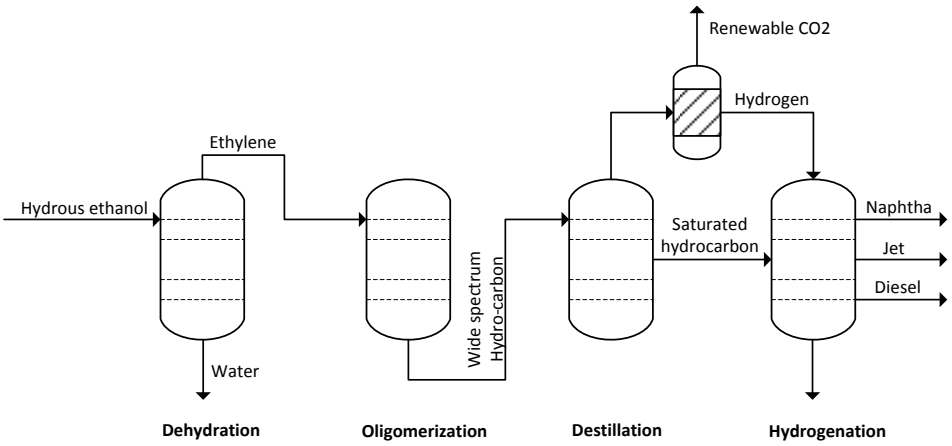

Figure 6.1: Steps of the alcohol to jet process (adapted from [226])

of biojet fuel (e.g. feed-in tariff and capital investment subsidy). The next section describes how the sugarcane-ethanol supply chain is conceptualized and formalized into a computational model, and how the aforementioned elements are added to this formalization.

6

6.2.2. CONCEPTUAL FRAMEWORK

A system diagram of the Brazilian biojet fuel supply chain is presented in Figure 6.2. The system is analyzed from the hypothetical viewpoint of the Brazilian government. This perspective is characterized by a government that aims to use the existing sugarcane-ethanol supply chain as a substrate for the emergence of a biojet fuel supply chain. The government's policy instruments are a capital investment subsidy and a feed-in tariff. We use these supply side policies because biojet fuel is in an early phase of introduction to the market and thus it is necessary to reduce the risk aversion of potential investors [228]. It is assumed that the behavior of the system is shaped by the external factors depicted in Figure 6.2.

Complex adaptive systems theory is used for the analysis of the phenomenon of the emergence of a Brazilian biojet fuel supply chain from the existing sugarcane-ethanol supply chain. This supply chain is considered as a complex adaptive system. This system consists of heterogeneous actors (farmers, sugar/ethanol producers) who constantly adapt their behavior (e.g. decision making about production and consumption of biofuels) in response to other actors' behavior and to changes in the environment (e.g. changing market prices).

The conceptualization of the system builds on the conceptual framework developed by Moncada *et al.* [167], which has been used in the analysis of the German biodiesel supply chain [190] and the Brazilian sugarcane-ethanol supply chain [225]. This framework describes a system by using concepts from complex adaptive systems theory and from the neo-institutional economics school of thought. The main tenet of this frame-

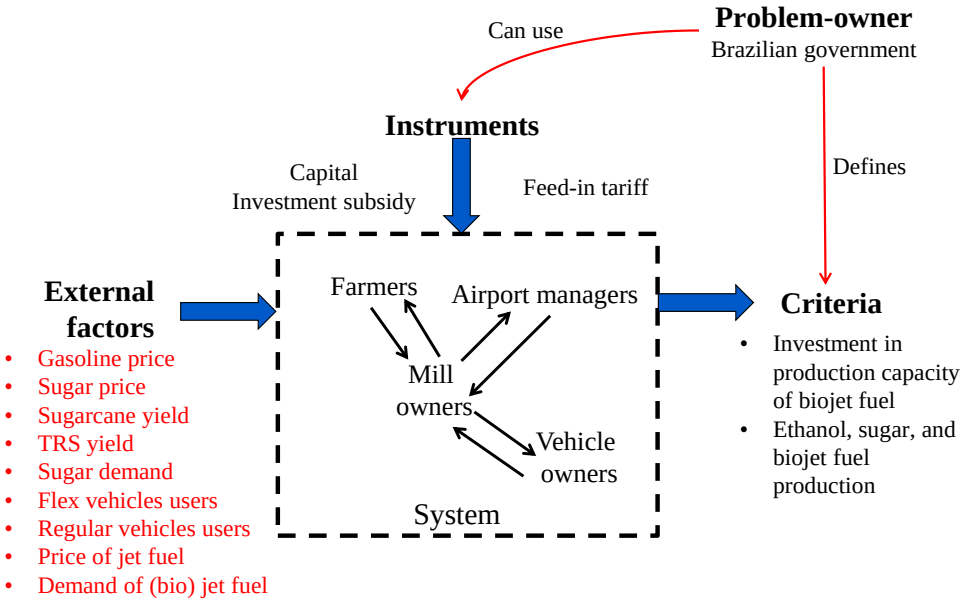

Figure 6.2: System diagram of the Brazilian sugar/ethanol and biojet fuel market.

work is that the state of the system at macro level (macro-behavior) emerges as a result of the interaction of three elements at micro level: the physical system, the network of actors, and institutions (see Figure 6.3).

The physical system specifies the physical objects in the system such as: farms, mills, vehicles, and airports. The actors are the entities that make decisions and perform a role in the system. In the biojet fuel supply chain, actors are farmers, mills/distillery owners, vehicle owners, and airport managers. Finally, institutions are the rules that structure social interaction [229]. Examples of institutions are: traditions, norms, legislation, policies, and governance structures.

Actors' behavior and the interaction among actors are governed by institutions at different levels. At the level of "games", institutions shape actors' behavior through heuristics and shared strategies that influence decision making. For instance, the selection of production ratios for sugar/ethanol/biojet fuel by mills owners is constrained by technical constraints and driven by profit maximization strategy. The level of institutional arrangements determines the interaction among actors. We use the CONSECANA-SP mechanism to describe the interaction between farmers and mills owners. We assume that the interaction between mills and vehicle owners and between mills and airports is governed by a supply-demand mechanism. Finally, the formal institutional environment refers to the rules of the game. Blending mandates for anhydrous ethanol in gasoline, taxes levied on hydrous and anhydrous ethanol are examples of institutions at this level in the Brazilian sugarcane-ethanol supply chain.

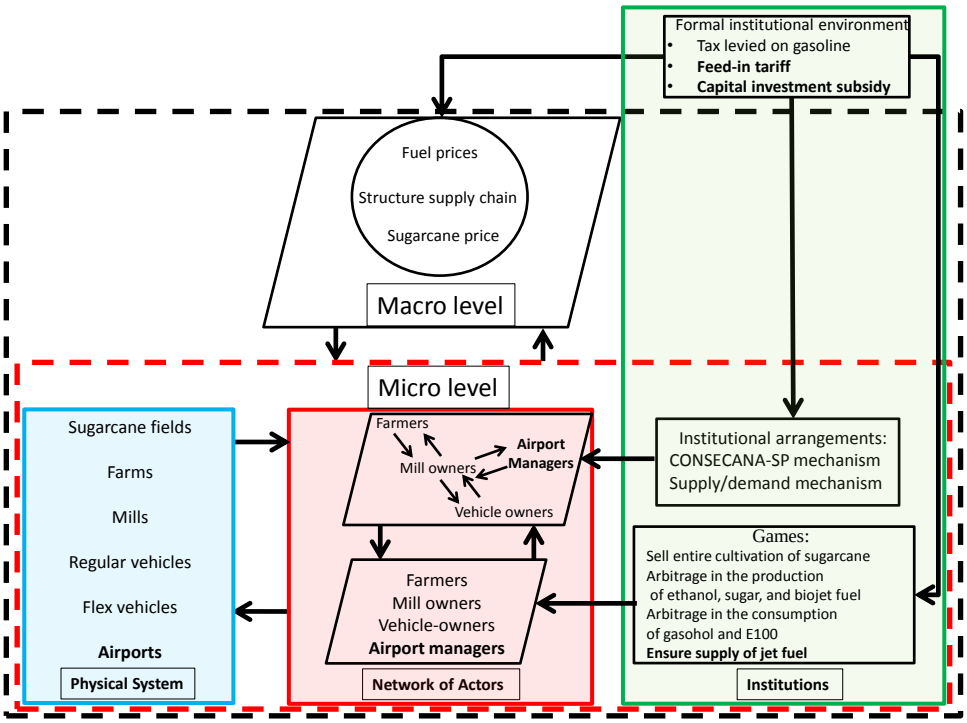

Figure 6.3: Conceptual framework. Elements in **bold** are the elements added to the Brazilian sugarcane-ethanol supply chain.

6.2.3. MODELLING FRAMEWORK

The conceptual framework is formalized into a computational model with the aim of analyzing the influence of the feed-in tariff, capital investment subsidy, and the tax levied on gasoline on the emergence of a biojet fuel supply from the existing sugarcane-ethanol supply chain. The selection of the model was based on the aim of the study. At the core of this aim is the concept of emergence. Emergence is defined as *"the arising of novel and coherent structures, patterns, and properties through the interactions of multiple distributed elements"* [47]. Agent-based modelling was chosen as the modelling paradigm as, unlike approaches such as general equilibrium modelling, supply chain optimization, and system dynamics, it enables one to describe a phenomenon in terms of unique and autonomous agents that interact with each other and the environment [37]. Moreover, agent-based modeling is arguably the most suitable tool for modeling a complex adaptive system because of its bottom up approach and easiness of including different formalisms into the model [48].

This study builds on a spatially-explicit agent-based model of the Brazilian sugarcane-ethanol supply chain [225]. This agent-based model uses land projections to explicitly account for expansion of land for sugarcane production in specific locations. These projections are provided by the PCRaster Land Use Change model (PLUC) [194]. The agent-

based model was designed using the pattern-oriented approach [168]. The model was structured based on three patterns: flexibility in the production of sugar/ethanol, flexibility in the consumption of ethanol, and the location of sugarcane availability. The model was implemented in NetLogo [124].

We extend the scope of that model by adding new actors (airports), new policies (feed-in tariff and capital investment subsidy), new technologies (biojet fuel production), and new considerations into the decision making about production and investment in processing capacity. With regards to production, mill owners need to decide how to allocate the sugarcane for the production of sugar, ethanol, and biojet fuel. With regards to investment, mill owners need to assess whether to invest in a conventional flex plant or to invest in a flex plant that includes the production of biojet fuel. Below, we describe in more detail the features added to the model. The description of the agent-based model is based on the ODD protocol proposed by Grimm *et al.* [195].

Purpose: the aim of the model is to study the influence of supply-side policies (i.e. feed-in tariff and capital investment subsidy) on the emergence of a biojet fuel supply chain in Brazil.

Entities, state variables and scales: The entities in the model are the actors in the supply chain: farmers, mill owners, car drivers, and airport managers. The farmers' main state variables are: farm area, sugarcane yield, and Total Recoverable Sugar (TRS) yield. The mills/distillery owners' main state variables are: type (flex plant, sugar plant, ethanol plant, or flex-biojet fuel plant), sugarcane processing capacity, production costs, and production ratio of sugar, ethanol, and biojet fuel. The drivers' main state variables are: vehicle type (flex vehicle, regular vehicle), energy demand, and preferences in the consumption of fuels[5]. The airports' main state variables are: total demand for jet fuel and the blending constraint for biojet fuel. Farmers and mills are modeled spatially explicitly, whereas drivers and airports are not. This is because the (bio)jet fuel, E100, and gasohol prices are considered uniform over space. The global environment consists of the policy instruments (feed-in tariff, capital investment subsidy, and gasoline tax), and the exogenous factors (annual world market prices of sugar and gasoline, number of flex and gasohol vehicles, sugar demand, sugarcane and TSR content yield, and price and demand of jet fuel). The temporal extent of the model is 18 years (2013-2030) and the time step is one year. The model is spatially explicit, covering the whole of Brazil. The input from PLUC to the agent-based model has a resolution of 5 x 5 km.

Process overview and scheduling: the process consists of a series of events that take place in discrete periods within a year. The process starts during the harvest season, where farmers *harvest sugarcane*, *negotiate* with the mills agents about price and quantity to be traded and *deliver the sugarcane* to the mill as it was agreed. As the interaction between farmers and mills agents is bound to their spatial location, these transactions are decentralized and take place at different locations.

Mill/distillery owners store the sugarcane and maximize profits *by deciding on volumes of sugar, hydrous ethanol, anhydrous ethanol, and biojet fuel to be produced* (Fig-

[5]The criterion for choosing ethanol (E100) as opposed to gasoline is the ratio of ethanol price to gasoline price. According to economic theory, this ratio should be less or equal to 0.7 as on average E100 is considered to deliver 70% of the mileage of gasoline for the same volume of fuel. In this study, however, we introduce heterogeneity in the value of this ratio to account for that some drivers have a preference for the consumption of ethanol even when this fuel is not the optimal choice.

ure 6.4). In each time period, mills/distillery owners *produce* sugar, ethanol, and/or biojet fuel and *enquiry about prices and quantities* of sugar and ethanol *to the sugar and fuel markets*. Drivers *choose between E100 and gasohol* based on relative prices. Airports *choose between biojet fuel and fossil fuel* based on market prices[6]. According to the market outlook, mills agents *decide about the expansion of the sugarcane processing capacity* to produce either sugar/ethanol or sugar/ethanol/biojet fuel. The new sugarcane processing capacity starts operation at the third year of construction. An overview of the model narrative and a description of some of the most important processes are presented in Appendix F.

Design concepts: the basic concepts underpinning the design of the agent-based model are presented below. The reader is referred to Moncada *et al.* [225] for a more comprehensive description of the concepts that guide the design of the agent-based model.

Basic principle: The basic principle applied in the model is the rational choice theory. This theory is used to describe the decision making on production of sugar, ethanol and biojet fuel.

Emergence: Emergent system dynamics includes gasohol and E100 prices, total production of sugar, ethanol, and biojet fuel, total demand for biojet fuel and jet fuel, and the expansion of the processing capacity of sugarcane.

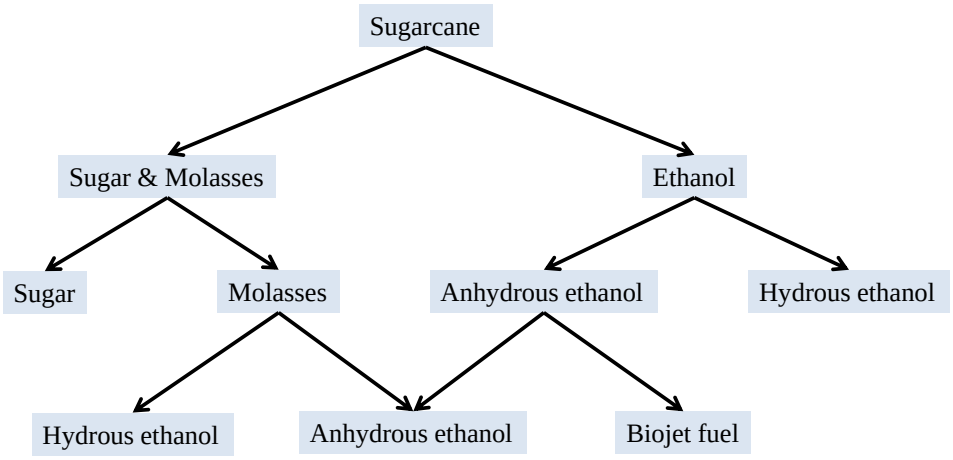

Figure 6.4: Levels of decision as to production of sugar, hydrous, anhydrous ethanol, and biojet fuel by the owners of flex plants. This decision making is based on market signals.

Adaptation: Flex mill owners and the drivers of flex vehicles are the entities that ex-

[6] In reality, the individual airline companies are the ones that decide whether to use jet fuel or biojet fuel. Nevertheless, we aggregated the demand of these airlines at the airport level for modeling purposes

hibit adaptive behavior in the model. The strategic behavior of drivers of flex vehicles and owners of flex mills is described in detail in Moncada *et al.* [225]. Owners of flex mills that also produce biojet fuel adapt their production ratios of ethanol/sugar/biojet fuel based on market signals (see Figure 6.4). This behavior is driven by a profit maximization strategy. Thus, high prices of sugar (or ethanol or biojet fuel) lead to an increase in the production of sugar (or ethanol or biojet fuel).

The decision of the flex mills about the volumes of sugar, ethanol, and biojet fuel to be produced is modeled as an optimization problem as presented below:

$$\underset{x_s, x_h, x_{hm}, x_{bj}}{\text{maximize}} \quad \sum_{i=1}^{4} \pi_i \tag{6.1a}$$

$$\text{subject to} \quad x_s >= x_{s_{min}} \tag{6.1b}$$

$$x_s <= 0.65 \tag{6.1c}$$

$$x_h >= 0.2 \tag{6.1d}$$

$$x_h <= x_{h_{max}} \tag{6.1e}$$

$$x_{hm} >= 0.2 \tag{6.1f}$$

$$x_{hm} <= x_{h_{max}} \tag{6.1g}$$

$$x_{bj} >= 0.1 \tag{6.1h}$$

$$x_{bj} <= 0.8 \tag{6.1i}$$

where π_i is the profit derived from product i (sugar, hydrous, anhydrous, and biojet fuel), x_s is the ratio of sugar production to sugarcane processed (the rest is used for ethanol production), x_h is the ratio of hydrous production to total ethanol production from sugarcane (the rest is used to produce anhydrous ethanol and biojet fuel), x_{hm} is the ratio of hydrous production to total ethanol production from molasses, x_{bj} is the ratio of biojet fuel production to total anhydrous ethanol production. $x_{s_{min}}$ is the minimum in the ratio of sugar production to sugarcane processed, $x_{h_{max}}$ is the maximum in the ratio of hydrous production to total ethanol production. Values for $x_{s_{min}}$ and $x_{h_{max}}$ differ among mills. To account for the influence of the gasoline tax on the decision making about the volumes of hydrous and anhydrous ethanol to be produced, it was assumed that $x_{h_{max}}$ is equal to one when gasoline tax is 2.46 R\$l^{-1} and that $x_{h_{max}}$ is equal to zero when the gasoline tax is 0 R\$l^{-1}. This assumption follows from the demand response. That is, a high gasoline tax will result in a major consumption of hydrous ethanol and thus will lead to an increase in the price of hydrous ethanol, which in turn will lead mill owners to increase the production of hydrous ethanol. A similar mechanism also applies to the effect of reducing the gasoline tax on the production of anhydrous ethanol.

Objectives: Flex mill owners are profit maximizing agents. They aim to maximize their profits by shifting the production ratio of sugar to ethanol and by shifting the production ratio of ethanol between hydrous ethanol, anhydrous ethanol, and biojet fuel. The production ratio of sugar to ethanol has to be between 35 percent and 65 percent because of a technical constraint [117]. Drivers of flex vehicles aim to meet their energy

demand by choosing between gasohol and E100. Farmers aim to sell their entire sugarcane cultivation to the owners of flex/distillery plants at the price determined by the CONSECANA-SP mechanism.

Learning/prediction: Mills forecast prices and demand for sugar, ethanol (hydrous and anhydrous), and biojet fuel. The forecasting is used to inform the decision making as to whether to invest in a new flex plant, to invest in a new flex plant with co-production of biojet fuel or to not invest at all.

Sensing: Farmers, owners of mills, drivers, and airport managers are assumed to know market prices (without uncertainty).

Interaction: The interaction between mills and drivers is mediated via the fuel market. This mechanism is described in detail in Moncada *et al.* [225]. Farmers directly interact with owners of mills/distilleries in their neighborhood through the negotiation about a contract for the supply of sugarcane. The main issue in the contract is the sugarcane price. This interaction is modeled through the CONSECANA-SP mechanism. Mills interact indirectly with neighboring mills by competing for contracts with farmers in their common sourcing region in the sugarcane market.

In the CONSECANA-SP mechanism the pricing of sugarcane is based on two variables: the amount of total recoverable sugar (TRS), and the price of TRS. The TRS price is linked to the average market selling prices of three different products (sugar, hydrous and anhydrous ethanol), over the period of one harvest season. The CONSECANA-SP model then assumes that sugarcane accounts for 59.5% of the production costs of sugar, and accounts for 62.1% of ethanol production [180]. In this study, we introduce a modification to the current CONSECANA-SP mechanism to account for the production of biojet fuel from sugarcane-ethanol. To simplify the analysis, this modification of the CONSECANA-SP mechanism neglects the contribution of naphtha and diesel in the determination of the sugarcane price. Accordingly, remuneration to suppliers is done according to these percentages.

$$P_s^{TRS} = \frac{0.595 P_s^{ave}}{sc_s} \tag{6.2}$$

$$P_h^{TRS} = \frac{0.621 P_h^{ave}}{sc_h} \tag{6.3}$$

$$P_a^{TRS} = \frac{0.621 P_a^{ave}}{sc_a} \tag{6.4}$$

$$P_{bj}^{TRS} = \frac{0.621 P_{BJ-a}^{ave}}{sc_a} \tag{6.5}$$

$$P_{BJ-a}^{ave} = P_{bj}^{ave} y_{BJ-a} \tag{6.6}$$

where P_s^{TRS}, P_h^{TRS}, P_a^{TRS}, and P_{bj}^{TRS} are the TRS prices for sugar, hydrous ethanol, anhydrous ethanol, and biojet fuel respectively, in Reais per kilogram of TRS. P_s^{ave}, P_h^{ave},

P_a^{ave}, and P_{bj}^{ave} are the average market selling prices for sugar, hydrous ethanol, anhydrous ethanol, and biojet fuel in Reais per kilogram of sugar, Reais per litre of ethanol, and Reais per liter of biojet fuel respectively. sc_s, sc_h, and sc_a are the stoichiometric coefficient for sugar, hydrous ethanol, and anhydrous ethanol, respectively. y_{BJ-a} is the yield of biojet fuel from anhydrous ethanol.

The TRS price for a processing plant i is based on weighing the product TRS price with the volumes of each product:

$$P_i^{TRS} = P_s^{TRS}\frac{Pr_s}{Pr_t} + P_h^{TRS}\frac{Pr_h}{Pr_t} + P_a^{TRS}\frac{Pr_a}{Pr_t} + P_{bj}^{TRS}\frac{Pr_{bj}}{Pr_t} \tag{6.7}$$

$$Pr_t = Pr_s + Pr_h + Pr_a + Pr_{bj} \tag{6.8}$$

Where P_i^{TRS} is the TRS price of the plant i in Reais per kg of TRS. Pr_s, Pr_h, Pr_a, and Pr_{bj} are the total production of sugar, hydrous ethanol, anhydrous ethanol, and biojet fuel of the plant i, respectively in kilograms of TRS.

Stochasticity: The model is initialized stochastically. Drivers' preferences of the relative fuel prices and mills' yields for sugar, hydrous ethanol, anhydrous ethanol, and biojet fuel are randomly assigned among the agents.

Collectives: The model neglects the formation of aggregations among individuals.

Observation: Expansion of the ethanol/sugar/biojet fuel production capacity, production of sugar, ethanol, and biojet fuel are the main key performance indicators.

Initialization: 418 mill agents, 3715 farmer agents, 2500 driver agents, and 40 airport managers are initialized for the year 2013. The location of mills and their type (sugar plant, ethanol plant, or flex plant) are based on real spatial data for the year 2013 [199]. Table 6.1 and Table 6.2 present the parameters that describe the state of the agents at the start of the simulation.

Input data: The behavior of the model is driven by 9 exogenous parameters: gasoline and sugar prices, number of flex and regular vehicles, productivity of both sugarcane and the TRS content, sugar demand, jet fuel price, and jet fuel demand. The productivity of both sugarcane and the TRS content is assumed to be constant during the period 2013-2030. The values for sugarcane yield and TRS content yield are 75 t ha^{-1} and 140 kgTRS, respectively. These values were set out based on historical developments [201]. Projections for the other parameters up to 2030 were retrieved from the literature (see Table 6.3).

The decision making about investment in processing capacity is based on the estimation of the Net Present Value. The values of the parameters used in the net present value calculation are reported in the Appendix G. It is assumed that mill owners have a different perception of risk in their investment decision. This difference in the perception of the risk was captured by using different values for the discount rate.

Critical assumptions that underpin the model structure are:

- The demand for (bio) jet fuel is perfectly inelastic.

Table 6.1: Farmers, vehicle users, and airports state variables and independent variables

Parameter	Value	Brief description	Units
		Farmers	
initial-number-farmers	3715	initial number of farmers	–
farm-a	2500	farm area	ha
yield-SC	75	yield of sugarcane per hectare	$t\,ha^{-1}$
yield-TRS	140	yield of total recoverable sugar per ton of sugarcane	$kg\,t^{-1}$
		Drivers	
Type		gasohol; flex	–
Demand	47244	energy demand per vehicle	MJ yr
preference-relative-price[a]	N(**0.9**, 0.1)	value in the relative price that determines the consumption pattern of the driver i. Values of the relative price higher than the individual relative price lead to consumption of gasohol by the driver	–
		Airports	
total-demand-jet-fuel	N.A	total demand of jet fuel. This demand can be satisfied either with jet fuel or partially satisfied with renewable jet fuel. This parameter depends on the projections for domestic demand of jet fuel in Brazil	$Ml\,yr^{-1}$
Blending constraint	30	Blending constraint of biojet fuel	%
		Independent variables	
blend-mandate[b]	23	blend mandate	%
tax-gasoline[b]	1.23	tax levied on gasoline	$R\$\,l^{-1}$
tax-hydrous[b]	0.30	tax levied on hydrous ethanol	$R\$\,l^{-1}$
tax-anhydrous[b]	0.05	tax levied on anhydrous ethanol	$R\$\,l^{-1}$
Feed-in-tariff	[3-6]	feed-in tariff for biojet fuel production	$R\$\,l^{-1}$
capital-investment-subsidy	[0-20]	governmental financial aid that covers a share of the total depreciable capital required to build a biojet fuel plant	%

[a] The value in **bold** was obtained from the model calibration (see Moncada *et al.* [225]).
[b] These values were retrieved from de Gorter *et al.* [171].

- Biojet fuel is only used in the jet fuel domestic market.
- There is no differentiation in the granting of feed-in tariffs.
- The supply curve of jet fuel is perfectly elastic.
- If there is price parity between biojet fuel and jet fuel, airports opt to first consume biojet fuel. Nevertheless, the demand of biojet fuel is restricted to the maximum blending constraint.

6.2.4. MODELLING OF THE POLICIES INCENTIVIZING PRODUCTION, CONSUMPTION, AND INVESTMENT IN BIOJET FUEL

In this study, we use two supply side policies: the feed-in tariff and the capital investment subsidy. A feed-in tariff is a policy instrument used to accelerate investments in renewable energy sources. This policy instrument offers long-term purchase agreements for the sale of renewable energy. The payment levels can be differentiated by the type of technology, resources, and location so as to better reflect production costs. In this study, we use the fixed feed-in tariff, which can be considered independent of the market price and we neglect any differentiation in the payment levels.

Let's consider the supply of jet fuel and biojet fuel as shown in Figure 6.5. If the payment level of the feed-in tariff is P_{FIT}, then the maximum supply to the fuel market is

Table 6.2: Mills state variables

Parameter	Value	Brief description	Units
		Mills	
number-sugar-mill-plants	10	number the sugar plants	–
number-ethanol mill plants	83	number of ethanol plants	–
initial-number-flex-mill-plants	325	number the mills plants	–
proc-capacity[a]	[1, 5]	processing capacity of sugarcane	$Mt\,yr^{-1}$
yield-sugar-SC[b]	U(119, 146)	yield of sugar per ton of sugarcane	$kg\,t^{-1}$
yield-hydrous-SC[b]	U(83, 92)	yield of hydrous ethanol per ton of sugarcane	$l\,t^{-1}$
yield-anhydrous-SC[b]	U(79, 88)	yield of anhydrous ethanol per ton of sugarcane	$l\,t^{-1}$
yield-biojet-fuel-SC[c]	U(35,42)	yield of biojet fuel per ton of sugarcane	$l\,t^{-1}$
yield-ethanol-molasses	U(8, 10)	yield of ethanol from molasses per ton of sugarcane	$l\,t^{-1}$
sugar-proc-cost	U(41, 51)	processing cost of sugar per ton of sugarcane	$R\$\,t^{-1}$
hydrous-proc-cost	U(14, 17)	processing cost of hydrous ethanol per ton of sugarcane	$R\$\,t^{-1}$
anhydrous-proc-cost	U(25, 31)	processing cost of anhydrous ethanol per ton of sugarcane	$R\$\,t^{-1}$
RJF-proc-cost	U(18,23)	processing cost of biojet fuel per ton of sugarcane	$R\$\,t^{-1}$
prod-ratio-sugar[d]	U(**0.5**, 0.6)	proportion of sugarcane that is used to produce sugar	–
prod-ratio-hydrous[d]	U(0.2,**0.5**)	proportion of sugarcane that is used to produce hydrous ethanol	–
prod-ratio-biojet-fuel	U(0.2-0.8)	proportion of sugarcane that is used to produce biojet fuel	–
prod-ratio-hydrous-molasses	U(0.2, 0.5)	proportion of ethanol produced from molasses that is used to produce hydrous ethanol	–

[a] The distribution of the production capacity was based on Valdes [200].
[b] It is assumed that the differences in the yields are due to differences in industrial efficiencies between mills/distilleries.
[c] Retrieved from Santos *et al.* [209]
[d] The values in **bold** were obtained from the model calibration (see Moncada *et al.* [225]).

Table 6.3: Definition of the exogenous parameters

Year	Sugar demand[a] [Mt]	Nominal sugar price[b] [US$kg^{-1}]	Nominal crude oil price[c] [US$bbl^{-1}]	Number Flex Vehicles[d] [millions]	Number Regular Vehicles[d,e] [millions]	Price jet fuel[f] [R$l^{-1}]	Domestic demand jet fuel[g] [Ml]
2013	34.85	0.39	104.08	23	15	2.20	2550.15
2014	35.92	0.37	96.20	26	14	2.03	2750.41
2015	36.94	0.30	50.80	28	13	1.07	2945.36
2016	37.88	0.40	42.80	30	13	0.90	3072.70
2017	38.76	0.40	55.00	32	13	1.16	3200.04
2018	39.58	0.40	60.00	35	13	1.27	3308.38
2019	40.33	0.40	61.50	37	13	1.30	3400.36
2020	41.01	0.40	62.90	40	13	1.33	3471.43
2021	41.63	0.39	64.50	43	13	1.36	3545.86
2022	42.19	0.39	66.00	46	13	1.39	3604.68
2023	42.67	0.39	67.60	49	14	1.43	3657.75
2024	43.09	0.39	69.30	53	14	1.46	3707.72
2025	43.45	0.39	71.00	56	14	1.50	3757.24
2026	43.74	0.39	72.80	59	14	1.54	3808.96
2027	43.97	0.39	74.60	62	15	1.58	3865.54
2028	44.13	0.38	76.40	66	16	1.61	3929.62
2029	44.22	0.38	78.20	69	17	1.65	4003.86
2030	44.25	0.38	80.00	73	17	1.69	4091.43

[a] The demand of sugar was calculated based on results reported by the MAGNET model [19].
[b] Retrieved from [202]. The ratio of domestic price of sugar to the international price is 1:1.2 [203].
[c] The ratio of crude oil price to gasoline price is 1:1.2 [204]
[d] Retrieved from [205, 206].
[e] Regular vehicles only can use gasohol (blend of gasoline and anhydrous ethanol. The maximum blend of anhydrous ethanol in gasohol is 27.5% v/v).
[f] The ratio of crude oil price to jet fuel 1:0.08 based on [230].
[g] It is assumed that the domestic demand amounts to 30% of the total demand of jet fuel. The projections of the total demand for jet fuel were retrieved from [226].

Q_{FIT}. The government offers a payment equivalent to P_{FIT} to the producers that bid biojet fuel until $Q_{bj} = Q_{FIT}$. Nevertheless, it is assumed that the government bids Q_{FIT} to the jet fuel market at the same price of the fossil jet fuel P_{FIT}.

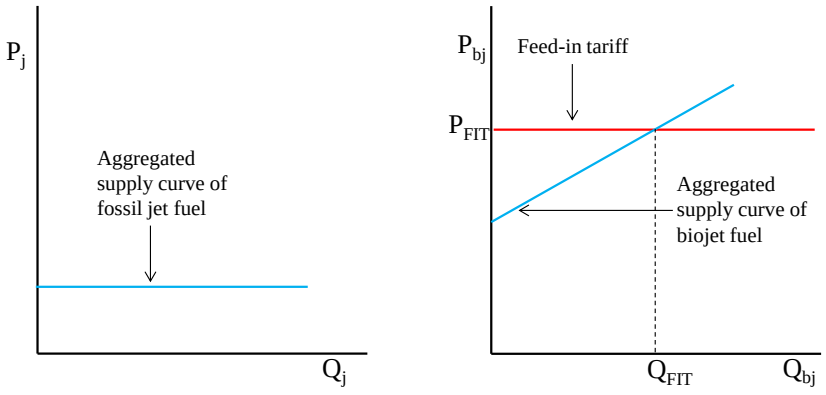

Figure 6.5: Hypothetical supply curves of jet fuel and biojet fuel.

Capital investment subsidy is a supply side policy used to incentivize investment in production facilities. This policy instrument aims to reduce the risk aversion of investors

by covering a percentage of the total fixed capital investment. In this study, we use capital investment subsidy as an instrument to only incentivize the production of biojet fuel. Thus, we add a cap in the production ratio of hydrous ethanol and a floor in the production ratio of biojet fuel to the plants that benefit from the capital investment subsidy. We assume a cap in the production ratio of hydrous ethanol of 0.5 (i.e. $x_h^{cap} = 0.5$) and a floor in the production of ratio of biojet fuel of 0.5 (i.e. $x_{bj}^{floor} = 0.5$).

6.3. RESULTS

IN this section, we describe the influence of the capital investment subsidy, the feed-in tariff, and the gasoline tax on two relevant aspects: the investment in sugarcane processing capacity[7] and the production of hydrous ethanol, anhydrous ethanol, and biojet fuel. We also present the influence of the feed-in tariff and capital investment subsidy on the subsidy costs. The results for investment in processing capacity and production of biofuels are presented in a matrix of 12 panels defined by the capital investment subsidy and the feed-in tariff. The results for the subsidy costs are presented in a matrix of 4 panels defined by the capital investment subsidy and the feed-in tariff. The gasoline tax or the type of biofuels is presented by different colors in each panel. The results presented below correspond to a tax levied on hydrous and anhydrous ethanol of 0.3 R$l^{-1} and 0.05 R$l^{-1}, respectively.

6.3.1. EVOLUTION OF SUGARCANE PROCESSING CAPACITY

Figure 6.6 shows the evolution of sugarcane processing capacity. There is a threshold in the investment in processing capacity: no investment, and thus no production of biojet fuel, takes place at a feed-in tariff of 3 R$l^{-1}. If the feed-in tariff is increased above 3 R$l^{-1}, there is an increase in investment in processing capacity. Nevertheless, the expansion of the processing capacity is almost brought to a halt in the year 2020 if the feed-in tariff is 4 R$l^{-1}. As an illustration, when comparing the scenarios with a capital investment subsidy of 20%, a feed-in tariff of 4 R$l^{-1}, and a gasoline tax of 0, 1.23, and 2.46 R$l^{-1}, the sugarcane processing capacity is 165, 93, 0 million tons in 2020 whereas is 208, 93, and 0 million tons in 2030, respectively. If the feed-in tariff is 6 R$l^{-1} and the tax levied on gasoline is equal or less than 1.23 R$l^{-1}, the expansion in processing capacity also evolves non-linearly. For instance, in the period 2020-2025, for a feed-in tariff of 6 R$l^{-1} and a capital investment of 20%, the investment in processing capacity grows 16.9% and 14.5% if the gasoline tax is 0 R$l^{-1} and 1.23 R$l^{-1}, respectively. This threshold is due to that values of the feed-in tariff below 4 R$l^{-1} are unable to outweigh the biojet fuel production costs.

The effect of the gasoline tax on the investment in sugarcane processing capacity hinges on the feed-in tariff. As the feed-in tariff increases the effect of the gasoline tax on the investment in processing capacity increases too. For instance, when comparing the scenarios with a gasoline tax of 0 R$l^{-1}, a capital investment subsidy of 20%, a feed-in tariff of 6 and 5 R$l^{-1}, the processing capacity is 1100 instead of 1000 in 2025. Tax free gasoline leads to increased investment in processing capacity. A reduction in the gasoline tax, at a high feed-in tariff, results in an increased investment in production capacity

[7] This sugarcane processing capacity includes the production of sugar, ethanol, and biojet fuel.

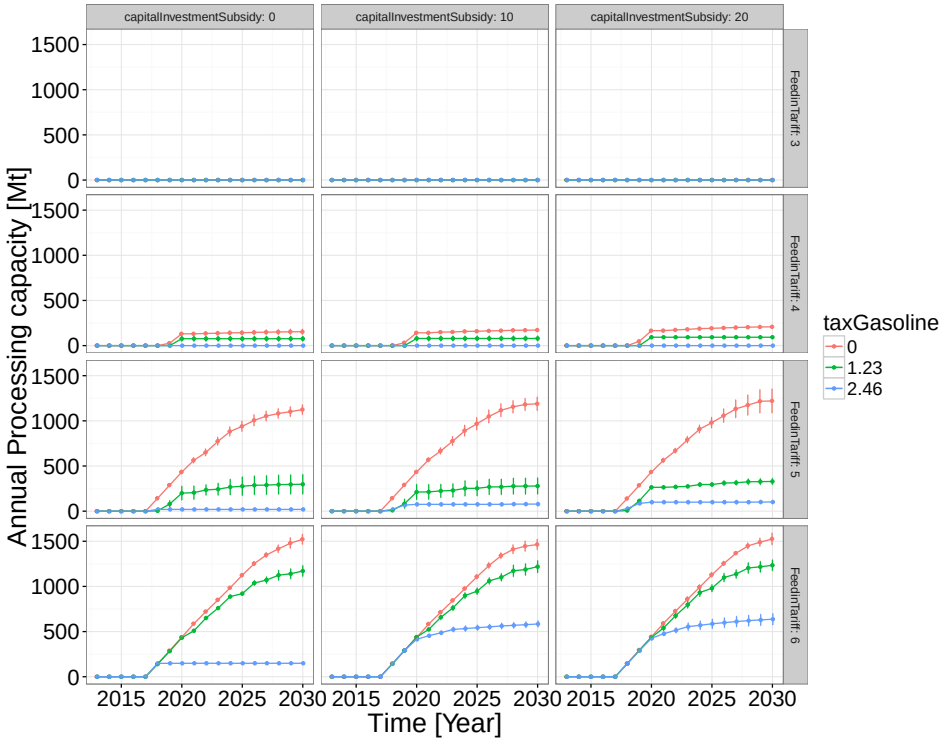

Figure 6.6: Sugarcane processing capacity of mills that include the production of biojet fuel for different combinations of the capital investment subsidy, feed-in tariff, and tax levied on gasoline. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff and gasoline tax in R\$l^{-1}. Blend mandate = 23%v/v, hydrous tax = 0.3 R\$l^{-1}, and anhydrous tax = 0.05 R\$l^{-1}.

because in this tax regime the demand for anhydrous ethanol increases. This increase in the demand for anhydrous ethanol leads to an increase in its price. The combination of high prices for anhydrous ethanol and high prices for biojet fuel (i.e. feed-in tariff) provide the right signals to investors. On the other hand, the effect of the capital investment on the investment in processing capacity is marginal.

6.3.2. PRODUCTION OF HYDROUS ETHANOL, ANHYDROUS ETHANOL, AND BIOJET FUEL

A tax free gasoline regime favors the production of anhydrous ethanol over hydrous ethanol and biojet fuel (see Figure 6.7). This pattern in the production of anhydrous ethanol is due to the assumption that owners of flex plants will only produce anhydrous ethanol if the gasoline tax decreases to 0 R\$l^{-1}. An increase in the feed-in tariff (above 3 R\$l^{-1}) leads to an increase in the production of hydrous ethanol and biojet fuel. When comparing the scenarios with a capital investment of 10% and feed-in tariff 5 and 4 R\$l^{-1}, the biojet fuel production is 2700 instead of 1000 Ml and the production of hydrous ethanol is 10 000 Ml instead of 6000 Ml in 2025. Also, the effect of the capital

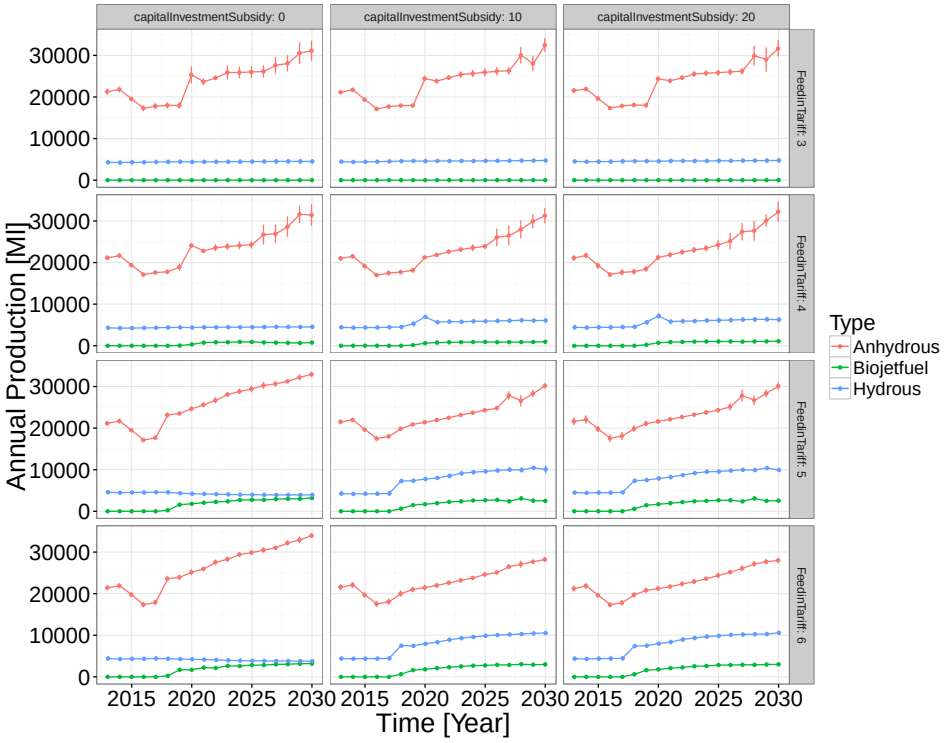

Figure 6.7: Production of hydrous ethanol, anhydrous ethanol, and biojet fuel for different combinations of the capital investment subsidy and feed-in tariff. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff in $R\$l^{-1}$. Gasoline tax = 0 $R\$l^{-1}$, blend mandate = 23%v/v, hydrous tax = 0.3 $R\$l^{-1}$, and anhydrous tax = 0.05 $R\$l^{-1}$.

investment subsidy on the production of biofuels depends on the feed-in tariff. At values of the feed-in tariff above 4 $R\$l^{-1}$, an increase in the capital investment subsidy leads to an increase in the production of hydrous ethanol and to a decrease in the production of both biojet fuel and anhydrous ethanol. For instance, when comparing the scenarios with a feed-in tariff of 5 $R\$l^{-1}$ and capital investment of 0 and 10%, the production of hydrous ethanol is 4000 instead of 8000 Ml, the production of biojet is 1800 instead of 1700 Ml, and the production of anhydrous ethanol is 25 000 instead of 21 000 Ml in 2020. This increase in the production of hydrous ethanol is due to the constraints in the production of hydrous ethanol and biojet fuel imposed on the plants that benefit from the capital investment subsidy. The mandate of producing a certain minimum of biojet fuel led to an optimal distribution of the production ratios that favors the production of hydrous ethanol. A further increase in the capital investment subsidy did not change the production patterns of hydrous and anhydrous ethanol, and biojet fuel. This is due to that the constraints in the production of hydrous ethanol and biojet fuel are assumed to be independent of the level of the capital investment subsidy. That is, the obligations imposed to the plants that received a subsidy of 10% is equal to the obligations imposed

to the plants that received a subsidy of 20%.

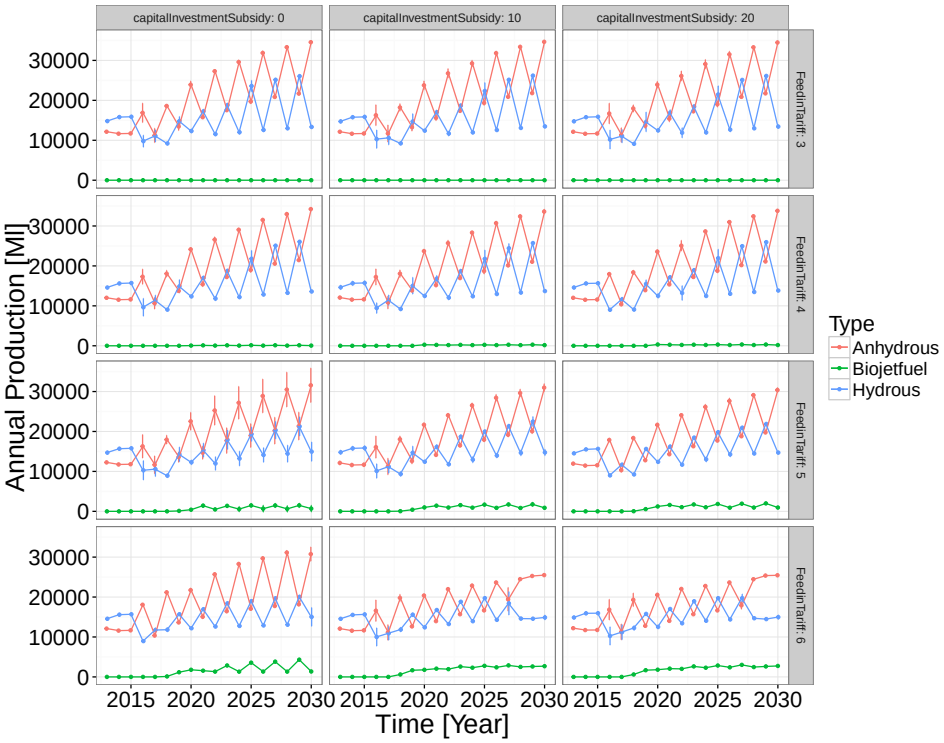

Figure 6.8: Production of hydrous ethanol, anhydrous ethanol, and biojet fuel for different combinations of the capital investment subsidy and feed-in tariff. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff in $R\$l^{-1}$. Gasoline tax = 1.23 $R\$l^{-1}$, blend mandate = 23%v/v, hydrous tax = 0.3 $R\$l^{-1}$, and anhydrous tax = 0.05 $R\$l^{-1}$.

As shown in Figure 6.8, there is an oscillating behavior in the production of hydrous and anhydrous ethanol if the tax levied on gasoline is 1.23 $R\$l^{-1}$. This behavior is the result of both the fuel choice of owners of flex vehicles that shifts between two states (i.e. consumption of either gasohol or hydrous ethanol) and the myopic behavior of the owners of the mills as to production of ethanol. This gasoline tax regime favors the production of anhydrous ethanol rather than hydrous ethanol. There is production of biojet fuel only if the feed-in tariff is equal to or greater than 4 $R\$l^{-1}$. The year of initial production of biojet fuel depends on the feed-in tariff. The supply chain starts producing biojet fuel in 2018 and 2020 if the feed-in tariff is 4 and 6 $R\$l^{-1}$, respectively. There is an oscillating behavior in the production of biojet fuel if the feed-in tariff is greater than or equal to 5 $R\$l^{-1}$. At a feed-in tariff of 5 $R\$l^{-1}$, the production of biojet fuel oscillates between 800 and 2000 millions of liters, whereas at a feed-in tariff of 6 $R\$l^{-1}$, the production of biojet fuel oscillates between 2000 and 3000 millions of liters. This oscillating behavior is also caused by the interaction of decision making between owners of flex vehicles and owners of mills about consumption of fuels and production of ethanol, respectively.

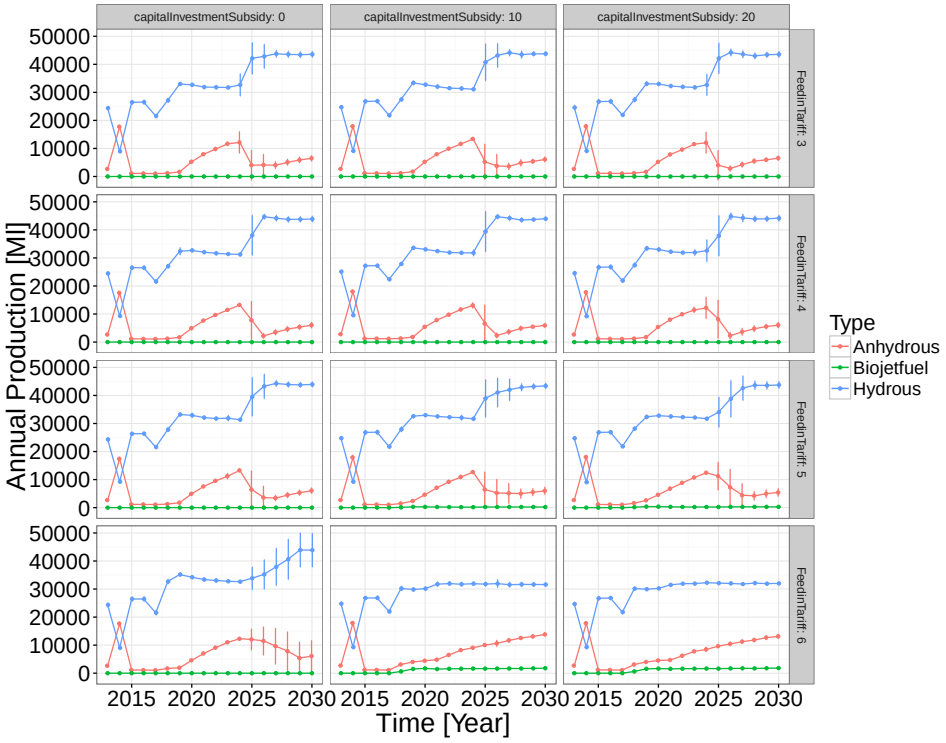

Figure 6.9: Production of hydrous ethanol, anhydrous ethanol, and biojet fuel for different combinations of the capital investment subsidy and feed-in tariff. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff in $R\$l^{-1}$. Gasoline tax = 2.46 $R\$l^{-1}$, blend mandate = 23%v/v, hydrous tax = 0.3 $R\$l^{-1}$, and anhydrous tax = 0.05 $R\$l^{-1}$.

In reality, this fast oscillation is unlikely to happen because actors adapt their behavior gradually. Nevertheless, the impact of this deviation of reality on the conclusions is negligible because this study focuses its analysis on extreme values in the gasoline tax (i.e. 0 and 2.46 $R\$l^{-1}$). At these values of the gasoline tax, decisions about the production and consumption of ethanol converge to one state (Figure 6.7 and Figure 6.9).

Figure 6.9 presents the evolution of the production of biojet fuel, hydrous, and anhydrous ethanol when the tax levied on gasoline is 2.46 $R\$l^{-1}$. These conditions favor the production of hydrous ethanol rather than anhydrous ethanol. Unlike the previous case when the gasoline tax is 1.23 $R\$l^{-1}$, biojet fuel is only produced at a feed-in tariff equal to or greater than 5 $R\$l^{-1}$ and a capital investment subsidy equal or greater than 10%. For instance, when comparing scenarios with a gasoline tax of 2.46 $R\$l^{-1}$, a capital investment subsidy of 20% and a feed-in tariff of 6 and 5 $R\$l^{-1}$, the production of biojet fuel is 1600 instead of 230 Ml in 2025. With regard to the production of hydrous and anhydrous ethanol, at a capital investment of 20% and a feed-in tariff of 6 $R\$l^{-1}$, the production of hydrous ethanol stays approximately constant at a value of 30 000 Ml as of 2020, whereas the production of anhydrous ethanol grows approximately 8% per year

in the period 2025-2030. This behavior in biofuels production is due to the constraints in the production of hydrous ethanol and biojet fuel imposed on the plants that benefit from the capital investment subsidy. In this case, the cap imposed in the production of hydrous ethanol favors the production of anhydrous ethanol and biojet fuel. The large standard deviations in the production of hydrous and anhydrous ethanol in 2024, 2025 and 2026 show that, although the surge in the production of hydrous ethanol is always present, its exact timing differs between these 3 years over the model runs.

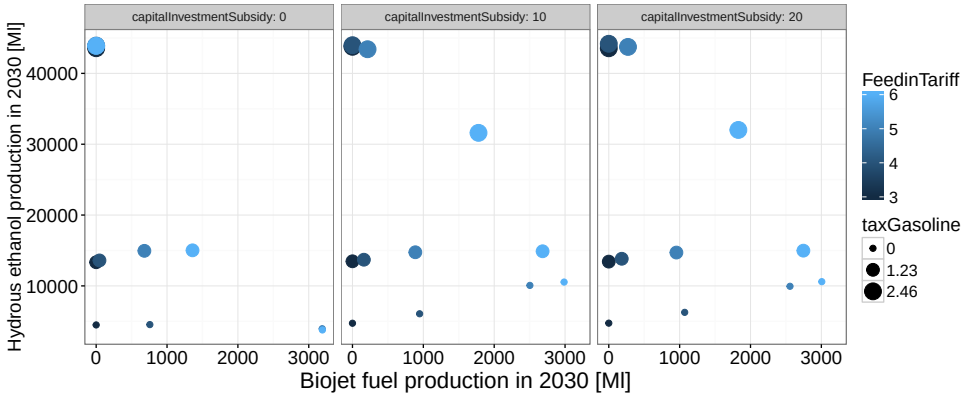

Figure 6.10: Production of hydrous ethanol and biojet fuel in 2030 for different combination of capital investment subsidy, feed-in tariff, and gasoline tax. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff and gasoline tax in R\$l^{-1}. Blend mandate = 23%v/v, hydrous tax = 0.3 R\$l^{-1}, and anhydrous tax = 0.05 R\$l^{-1}.

Figure 6.10 presents the trade-offs between the production of hydrous ethanol and biojet fuel in the year 2030. Patterns in biojet fuel production in 2030 hinge on the interaction of gasoline tax, capital investment subsidy, and the feed-in tariff. In a tax-free gasoline regime, an increase in the feed-in tariff results in an increase in the production of biojet fuel. The effect of the capital investment subsidy on the production of biojet fuel is characterized by a threshold. Excepting for the regime of free-tax gasoline in combination with high feed-in tariffs, the production of biojet fuel increases when the capital investment subsidy is higher than zero. Nevertheless, a further increase in the capital investment subsidy does not further incentivize the production of biojet fuel. This is due to the assumption that the constraints in the production of hydrous ethanol and the mandates in the production of biojet fuel are independent of the level of the capital investment subsidy. Overall, in this regime an increase in the feed-in tariff favors the production of both hydrous ethanol and biojet fuel.

At a tax level of gasoline of 1.23 R\$l^{-1}, the production of biojet fuel in 2030 increases with an increase in the feed-in tariff. At this level of the gasoline tax, no trade-offs exist between production of hydrous ethanol and biojet fuel: an increase of the feed-in tariff leads to higher production of biojet fuel without compromising the production of hydrous ethanol. The effect of the capital investment subsidy on the production of biojet fuel is similar to the one described for the tax-free gasoline regime.

At a tax level of gasoline of 2.46 R\$l^{-1}, the production of biojet fuel in 2030 increases

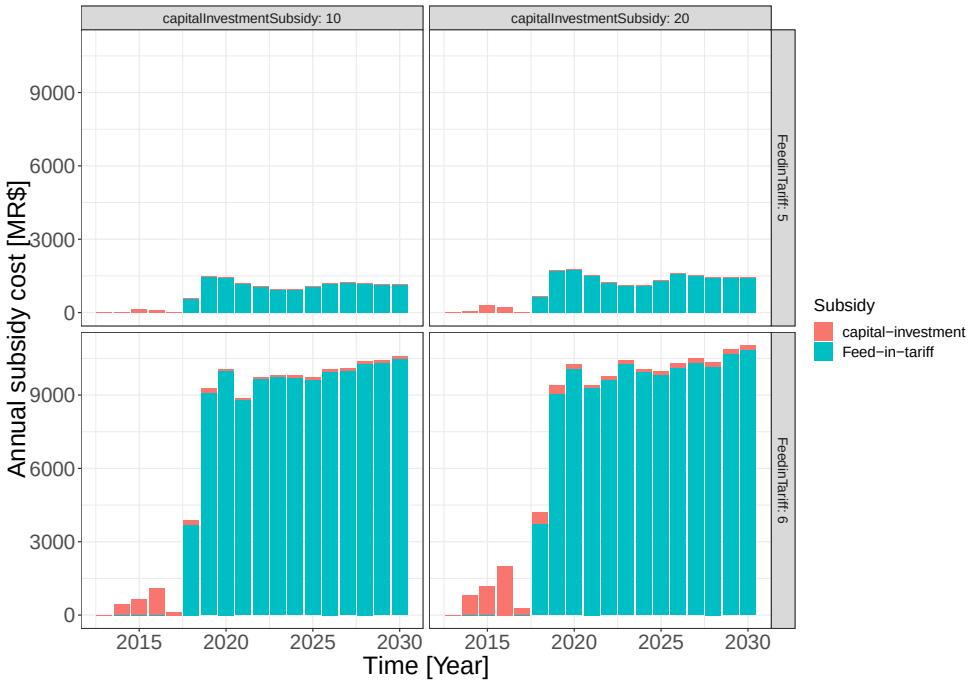

Figure 6.11: Evolution of the subsidy cost to spur the emergence of a biojet fuel supply chain at a gasoline tax rate of 2.46 Rl^{-1}. Capital investment subsidy as a percentage of the total depreciable capital for investment in a biojet fuel plant. Feed-in tariff and gasoline tax in Rl^{-1}

with an increase in the feed-in tariff if the capital investment subsidy is greater than or equal to 10%. At this level of taxation on gasoline, the effect of the capital investment subsidy on the production of biojet fuel is characterized by a threshold. In this regime, the production of biojet fuel only increases when the capital investment subsidy is higher than zero. This regime is also characterized by a trade-off between the production of hydrous ethanol and biojet fuel. At a capital investment greater than 0%, feed-in tariffs below 6 Rl^{-1} lead to largely the production of hydrous ethanol, whereas a feed-in tariff of 6 Rl^{-1} leads to an increase in the production of biojet fuel and to a decrease in the production of hydrous ethanol.

All in all, for a feed-in tariff above 4 Rl^{-1}, the gasoline tax exhibits an inversely correlated effect on the production of biojet fuel. That is, the higher the gasoline tax the lower the biojet fuel production. This is due to that a high gasoline tax results in an increase in the demand and thus, in an increase in the price of hydrous ethanol. These conditions favors the production of hydrous ethanol. Nevertheless, provided that there are mechanisms that ensue the production of biojet fuel as in this case the capital investment subsidy, the production of biojet fuel (1800 Ml) in 2030 at a gasoline tax rate of 2.46 Rl^{-1} is sufficient to satisfy the domestic demand of jet fuel (4000 Ml) in 2030 because of the blend wall, defined as blending biojet fuel into jet fuel at 30%.

The cost of subsidizing the emergence of a biojet fuel supply chain under different

combination of the capital investment subsidy and feed-in tariffs at a gasoline tax rate of 2.46 R$l^{-1} is presented in Figure 6.11. The most significant contribution in costs to spur biojet fuel production comes from a feed-in tariff of 6 R$l^{-1} with a cost of approximately 9000 MR$ per year as of 2020. The contribution of the capital investment subsidy is notably in 2016 with a value of approximately 1500 MR$. The general subsidy cost pattern is characterized by the early introduction of the capital investment subsidy followed by a cost regime dominated by the feed-in tariff.

6.4. DISCUSSION

THE results suggest that the emergence of a Brazilian biojet fuel supply chain, from the existing sugarcane-ethanol supply chain, is largely driven by a tax-free gasoline regime and a feed-in tariff greater than 3 R$l^{-1} (see Figure 6.6 and Figure 6.10), provided that the policy landscape for both road transport and aviation sector remains stable, that the demand for (bio)jet fuel is perfectly inelastic, that there is no differentiation between the type of technologies, resources, and location in the granting of feed-in tariffs, and that the effect of import and export tariffs on the market is negligible. We also found that the effect of the capital investment subsidy on sugarcane processing capacity is negligible. These findings are in line with the reported by Del Rio and Bleda who point out the advantages of feed-in tariff to lower risks in renewable energy investment [231].

The results also suggest that the production patterns of biojet fuel are heavily influenced by the gasoline tax (see Figure 6.7 - Figure 6.9). A tax-free gasoline regime favors the production of biojet fuel even when the capital investment subsidy is zero. That is, even in situations where the constraint for hydrous production and the mandate for biojet fuel production imposed on the plants that receive the capital investment subsidy were absent. Unlike the tax-free gasoline regime, an increase in the level of taxation of gasoline requires mandates for the production of biojet fuel to ensure its production. Whilst changes in the values assumed for the cap and floor in the production ratio of hydrous ethanol and biojet fuel, respectively, will bring about different absolute production quantities for the three fuels, the production patterns of biojet fuel will remain qualitatively similar.

We found that there is a trade-off between the production of hydrous ethanol and biojet fuel in 2030 at high levels of taxation of gasoline (see Figure 6.10). This insight may be relevant for a Brazilian government that strives for the decarbonisation of both the road transport sector and the aviation sector. Our results suggest that increasing the level of gasoline taxation, a feed-in tariff of 6 R$l^{-1}, and introducing regulations in the production of biojet fuel through mechanisms as the capital investment subsidy increases the production of hydrous ethanol without compromising the production of biojet fuel, if the sugarcane-ethanol supply is used to support the emergence of a biojet fuel supply chain. In fact, the biojet fuel produced at a gasoline tax rate of 2.46 R$l^{-1}, a feed-in tariff of 6 R$l^{-1}, and a capital investment subsidy of 10% is sufficient to satisfy 30% of the domestic demand (blend wall). Our results also suggest that the feed-in tariff has the most significant contribution in the costs to spur biojet fuel production (see Figure 6.11).

Biojet fuel is considered a cornerstone in the strategy to achieve the GHG emissions

reduction targets[8] of the aviation sector. Spurring the production and consumption of biofuels requires specific policies at the national and international level. At the national level, we showed in this study what policy instruments are necessary to enable the emergence of a biojet fuel supply chain from the existing sugarcane-ethanol supply chain. At the international level, government, industry and civil society representatives reached an agreement on a global market-based measure (GMBM) to reduce aviation carbon emissions through offsetting. Nevertheless, it is unclear whether this market mechanism will drive the development of biojet fuel supply chains. The model developed in this study could be coupled with models developed to describe other biomass and biofuels markets in different geographies via a multi-model ecology framework[9] [232]. Thereby, we can account for the inherently international nature of the aviation sector and provide insights as to the effect of market mechanisms on the deployment of biojet fuel supply chains.

Our study applies a number of key enhancements to the exploration of the emergence of a biojet fuel supply chain. First, to the best of our knowledge, this is the first study that provides insights into how different policy instruments may steer the emergence of a biojet fuel supply chain. Previous analyses are qualitative and thus only offer a description of the phenomenon of emergence, not a quantification [233]. Second, this is the first work that shows how the sugarcane-ethanol supply chain can be used as a platform for the emergence of a biojet fuel supply chain.

Our study also applies a number of key enhancements to the agent-based modelling of the Brazilian ethanol supply chain [225]. First, it modifies the CONSECANA-SP mechanism to account for the production of biojet fuel. Second, it adds the option of investing in biojet fuel production. Finally, it incorporates the feed-in tariff and the capital investment subsidy into the analysis.

From the methodological viewpoint, we have shown how a modeller can use the conceptual framework developed by Moncada *et al.* [167] and the ODD protocol to build an agent-based model to explore the emergence of a biojet fuel supply chain. The advantage of using the conceptual framework is that offers a systematic method to identify social processes, theories and structures that underlie the model's design. That is, the conceptual framework identifies the elements that one needs to consider for the modelling of a biofuel supply chain such as: actors' decision making and interaction, social structures, and the effect of policies on actors' behaviour. This is considered useful in the light that current biomass/biofuels markets models neglect the effect of social processes, differences between individual actors, and social structures on the evolution of the system. As we showed in this study, these processes play an important role in the emergence of a biojet fuel supply chain.

This approach, however, does have some limitations. First, we limit our analysis to the use of supply side policies granted by the Brazilian government. We neglect the introduction of any market mechanism[10] to stimulate the production of biojet fuel driven by the goal to improve the greenhouse gas emissions performance. These market mech-

[8] The Air Transport Action Group (ATAG) has established goals to reach carbon neutral growth from 2020 and reduce net carbon dioxide emissions by 50% (relative to 2005 levels) by 2050.

[9] Multimodel ecology is defined as *"an interacting group of models coevolving with one another in a dynamic sociotechnical environment"* [232]

[10] A market mechanism refers to the process whereby the market solves resource allocation problems.

anisms may become relevant to the decarbonisation of the aviation industry as this sector is inherently international. Second, given the scope of this study, we neglect the interaction of the production of biojet fuel by the alcohol-to-jet fuel pathway with other potential production routes (e.g. hydro-processed esters and fatty acids (HEFA), direct fermentation sugars-to-hydrocarbons (DFJ), biomass gasification and Fischer-Tropsch syngas-to-jet (GFT)). Indeed, the emergence of biojet fuel supply chains is largely the result of both the collaboration among the stakeholders in the supply chain and the competition for resources with actors who use different technologies or with actors in other sectors. Finally, we neglect the contribution of co-products in biojet fuel production (i.e. diesel and naphtha) in the determination of sugarcane price through the CONSECANA-SP mechanism. Discussions among farmers, sugar/ethanol producers, and potential biojet fuel producers, on how to account for the influence of biojet fuel production and co-products in the pricing of sugarcane, may hinder or speed up the development of the biojet fuel supply chain in Brazil. Finally, we neglect the effect of the electricity market (i.e. electricity prices) on the producers' decision making as to production of sugar, ethanol, and biojet fuel.

Yet, this study provides new insights into the emergence of a Brazilian biojet fuel supply chain under different policy landscapes. A further step would be to incorporate the on-going discussion about the biofuel policy in Brazil into the analysis, namely, the creation of a market mechanism that aims for the reduction of greenhouse gas emissions by rewarding the production of cleaner biofuels.

6.5. CONCLUSIONS

THIS study was conducted to answer the following research question: *Under what institutional conditions (i.e. formal policies) may the biojet fuel supply chain emerge in Brazil in the period 2015-2030?* To answer this question, we extended an agent-based model of the Brazilian sugarcane-ethanol supply chain to analyze the influence of the feed-in tariff, capital investment subsidy, and gasoline tax on the emergence of a biojet fuel supply chain.

The emergence of a biojet fuel supply chain from the existing Brazilian sugarcane-ethanol supply chain hinges on the interaction of the feed-in tariff and the gasoline tax. In a tax-free gasoline regime, a feed-in tariff above 3 R\$l^{-1} stimulates the production of biojet fuel. Nevertheless, at higher levels of gasoline taxation (i.e. 2.46 R\$l^{-1}), any feed-in tariff is insufficient to ensure the production of biojet fuel. Thus, at these levels of taxation of gasoline it is necessary to introduce regulations on the production of biojet fuel to ensure its production. We also found that the influence of capital investment subsidy on the emergence of a biojet fuel supply chain is significant at high levels of gasoline tax. At these levels of gasoline tax, it is the capital investment subsidy and its mandate as to the production of biojet fuel that sows the seed for the emergence of a biojet fuel supply chain and ensures a minimum in the biojet fuel production, respectively. Finally, we found that the feed-in tariff has the most significant contribution in the costs to spur biojet fuel production.

Using the existing sugarcane-ethanol supply chain as a platform for the emergence of a biojet fuel supply chain poses a policy dilemma as to the decarbonisation of the transport sector. Namely, the trade-off between hydrous ethanol and biojet fuel production.

One way out of this dilemma is to increase the level of gasoline taxation and to introduce regulations on the production of biojet fuel to ensure its production. We showed that under these institutional conditions, the production of biojet fuel is sufficient to satisfy 30% of the domestic demand of jet fuel (blend wall) in 2030 provided that the domestic demand amounts to the 30% of the total demand. Nevertheless, given the international nature of aviation and that there is major local control over road transportation, it is expected that policies are designed and implemented to spur the production of biofuels in the road transport sector.

All in all, this study is a step forward in understanding the phenomenon of emergence of biofuel supply chains. Here, we show how this phenomenon can be explored by both conceptualizing the system as a complex adaptive system and formalizing this conceptualization into an agent-based model. We also show how the existing sugarcane-ethanol supply chain can be used as a substrate for the emergence of a biojet fuel supply chain. Finally, we show how the conceptual framework used in this study provides a systematic method to identify social processes and structures that underlie the model's design. Notwithstanding the importance of these processes and structures in the evolution of (bio)energy systems, these elements are neglected by mainstream approaches.

The inherently international nature of the aviation sector poses a serious challenge in the analysis of the evolution of biojet fuel supply chains. To provide a better description of this phenomenon, it is necessary to account for the interaction of biomass/biofuels markets at the national and international level as well as the developments of global market forces. As it is impossible to capture all of the complexity of socio-technical systems in one single model, we recommend integrating models that describe biomass/biofuel markets in different geographies to provide insights into how biojet fuel supply chains may evolve. The multimodel ecology approach may be useful to facilitate model integration.

Finally, we recommend further research into the effect of an unstable policy landscape for the road transport on the evolution of a biojet fuel supply chain. Moreover, given the current debate about the future direction of the biofuel policy in Brazil, we recommend further research into the effect of market mechanisms based on greenhouse gas emissions on the emergence of a Brazilian biojet fuel supply chain.

7

CONCLUSION

There are more things in heaven and earth, Horatio,
Than are dreamt of in your philosophy.

William Shakespeare, *Hamlet*

7.1. OVERVIEW

BIOFUELS can play an important role in the transition towards a more sustainable energy system. The potential contribution of biofuels to decarbonize the energy system, however, depends on both governmental support and the effectiveness of the policy analysis and design. Optimization/equilibrium models are increasingly being used to assist in the policy analysis and policy design supporting the expansion of biofuel supply chains. These models have provided insights as to the location and scale of biofuel production plants and the environmental performance of biofuel supply chains. Nevertheless, these models are unable to shed light on the mechanisms that lead to the emergence of a biofuel supply chain. This incapacity of describing the phenomenon of emergence is due to either the assumption of static equilibria or the assumption that the predetermined system structure governs the dynamics of the system.

Understanding the phenomenon of emergence of a biofuel supply chain can inform policymakers in designing policy instruments to spur the production and consumption of biofuels. Once it is understood how biofuel supply chains may come into being, policymakers can stimulate the development of biofuel supply chains by tweaking the technological, economic, and institutional conditions.

This motivated us to formulate our research question as follows:

- *Given certain technological conditions and resources available, what institutional conditions are conducive to the emergence of a biofuel supply chain?*

In this research, we developed a formal method for analysis of biofuel supply chains that incorporates the interaction of social processes with processes governed by the laws of nature. This formal method consists of (i) a conceptual framework and (ii) its formalization into an agent-based model. We used this formal method to simulate the evolution of the German biodiesel supply chain, the Brazilian sugarcane-ethanol supply chain, and the hypothetical emergence of a biojet fuel supply chain in Brazil.

The conceptual framework builds on concepts from Complex Adaptive Systems (CAS) theory, Socio-Technical Systems (STS) theory, and Neo-Institutional Economics (NIE) school of thought (see Chapter 2). Concepts from STS theory and NIE school of thought such as physical system, network of actors, and institutions constitute the building blocks of the conceptual framework. Based on the CAS theory, the framework distinguishes two levels of behavior: the micro-level and the macro-level. The behavior at the macro-level is the aggregate system behavior that emerges from all interactions at lower levels in the physical system, the network of actors, and institutions. The micro-level refers to the rules and state variables that describe the behavior of those components. The framework was developed with the aim of both conceptualizing the evolution of a biofuel supply chain and guiding the design of agent-based models of biofuel supply chains.

Through case studies, we provide evidence that this formal method enables us to incorporate actors' preferences in their decision making, governance structures, and fiscal policies into the design of the agent-based model (see Chapter 3 - Chapter 5), as well as to analyze the effect of supply side policies on the emergence of a biofuel supply chain (see Chapter 6). Overall, the outcomes of this research contribute to enhance our understating of the effect of formal institutions on the evolution of biofuel supply chains.

The remainder of the chapter is organized as follows: Section 7.2 presents the main outcomes of this research. A reflection on the process and outcomes of this research is presented in Section 7.3. Section 7.4 describes the lessons learnt in this research. Finally, Section 7.5 discusses the recommendations for further research.

7.2. RESEARCH OUTCOMES

We have answered the main research question by addressing the following research sub-questions:

1. What patterns in existing biofuel production and production capacity are generated as result of actors' behavior?

2. What patterns in existing biofuel production and production capacity emerge from different types of policy interventions?

3. What institutional conditions are conducive to the emergence of a biojet fuel supply chain from an existing road transport biofuel supply chain?

The research sub-questions will be discussed in the next three subsections:

7.2.1. WHAT PATTERNS IN EXISTING BIOFUEL PRODUCTION AND PRODUCTION CAPACITY ARE GENERATED AS RESULT OF ACTORS' BEHAVIOR?

To answer this research sub-question, we used the conceptual framework along with the MAIA[1] framework to build an agent-based model of the German biodiesel supply chain. The model sheds light on the influence of actors' behavior on volumes of biodiesel produced and investment in production capacity.

We found that the dynamics of production capacity observed in Germany in the period 2000-2014 can be explained by the hypothesis that these patterns emerge from investors basing their decisions on optimistic perceptions of the market development. Patterns in production of biodiesel, however, cannot be completely explained with this hypothesis because of increasing imports of rapeseed and biodiesel from 2006 onwards, which were not included in the model. Thus, we recommended analyzing the effect of the interaction of the global rapeseed and vegetable oil markets with the German biodiesel supply chain on biodiesel production (see Chapter 3).

We also found that the assumption that all biofuel producers have the same perception of market development is robust, which is in line with the process of stabilization and convergence of actors' expectations presented in the strategic niche management framework (see Chapter 3).

In this case study, we showed how the formalization of the conceptual framework into an agent-based model can be used to test hypotheses that aim to explain the phenomenon of interest. This is considered useful in the light that mainstream modelling approaches are unable to provide insights about what mechanisms are relevant to explain the phenomenon. This formalization of verbal models into an agent-based model has important implications for policy making to spur biofuel supply chains. As these systems are complex and our understanding of social and economic phenomena is still limited, it can be particularly helpful to use agent-based modelling to formalize and provide insights into the mechanisms at work in a biofuel supply chain.

7.2.2. WHAT PATTERNS IN EXISTING BIOFUEL PRODUCTION AND PRODUCTION CAPACITY EMERGE FROM DIFFERENT TYPES OF POLICY INTERVENTIONS?

Two case studies were analyzed to answer this research sub-question: the production of biodiesel in Germany and the production of sugarcane-ethanol in Brazil. In the case of the German biodiesel supply chain, we used the agent-based model developed to answer the aforementioned research sub-question. The model was used to provide insights into what alternative stories (scenarios) could have unfolded as a result of different policy interventions in Germany. The model was also used to analyze the impact of the biodiesel tax and penalty on patterns in biodiesel production and adoption of rapeseed by farmers. Finally, the model was used to analyze the effect of agents' adaptation mechanisms to forecast prices on patterns in biodiesel production.

We found that the timing of policy interventions (agricultural and biofuel policies) matters in the evolution of the system. An early (late) liberalization of the agricultural market leads to a under production of biodiesel (collapse of the market). Hence, to stim-

[1] **M**odelling **A**gent systems using **I**nstitutional **A**nalysis

ulate production of biodiesel, the agricultural market should be enacted within a policy window. On the other hand, an early introduction of the biodiesel tax leads to stagnation in biodiesel production and investment in production capacity. A late introduction of the tax leads to an increase in sunk costs provided that the biofuel quota is binding. Furthermore, we found that patterns in biodiesel production and rapeseed adoption hinge on the policy regime and its dominant policy instrument. When the biodiesel tax is the dominant policy instrument biodiesel production and rapeseed adoption patterns decrease following an increase in the level of taxation (see Chapter 4).

We also found that in the event that an external shock (e.g. the introduction of a new policy) is introduced in the system, actors' adaptation mechanisms to changes in prices heavily influence the production of biodiesel (see Chapter 4). This finding suggests that individual behavior influences system behavior. This insight might assist the design of policies to spur the emergence of new biofuel supply chains by making clear the mapping from design variables to design objectives. As an illustration, we found that the robustness in biodiesel production (design objective) depends on the actors' adaptation mechanism. As, in turn, the adaptation mechanisms are a function of the information available to actors (design variables), this finding implies that the design of mechanisms that improve the accessibility of pertinent information to actors may contribute to the robustness of the system.

In the case of the Brazilian ethanol supply chain, we used the conceptual framework along with the ODD[2] protocol to build a spatially-explicit agent-based model of the Brazilian sugarcane-ethanol supply chain. The aim of the model was to explore the effect of biofuel policies (i.e. blending mandate, taxes levied on ethanol and gasoline) on the supply chain behavior.

This agent-based model applies a number of key enhancements to prior studies. First, it models the expansion of the sugarcane processing capacity in Brazil spatially-explicit, as the investment decision making in new sugarcane processing capacity is bound to the land availability and location. Second, it incorporates the CONSECANA-SP mechanism to model the interaction between farmers and producers. Finally, it includes preferences in and variation between the decision making of consumers. Overall, these characteristics have been neglected in previous studies to ensure mathematical tractability and rigor. As we showed in this research, these elements and their interaction are necessary to produce system behavior.

We found that under the set of chosen policy measures, the expansion of the sugarcane processing capacity is driven most by a high gasoline tax. The effect of the blend mandate on the investment in processing capacity is negligible when the gasoline tax is high. The pattern of expansion shows an east to west pattern, from Sao Paulo state to Goiás, Mato Grosso, and Mato Grosso do Sul. We also found that the consumption pattern of the owners of flex vehicles hinges on the interaction among gasoline prices and taxes levied on gasoline. That is, the gasoline tax exhibits a correlated effect on E100 demand. Blend mandates have a negligible influence on consumption patterns. Finally, we found that an increase in the gasoline tax leads to an increase in the production of hydrous ethanol and to a decrease in the production of anhydrous ethanol. The tax levied on hydrous ethanol influences the production patterns of ethanol at conditions other

[2] **O**verview, **D**esign concepts, and **D**etails

than gasoline tax-free. In these conditions, an increase in the hydrous ethanol tax leads to a decrease in the production of hydrous ethanol and leads to an increase in the production of anhydrous ethanol. These production patterns of ethanol are independent of the blend mandates. Taxes on anhydrous ethanol have no impact at all (see Chapter 5).

Given that the Brazilian government aims to increase the consumption of hydrous ethanol in the energy mix in 2030, and thus needs to double the supply of ethanol, our findings suggest that this goal is achievable if the gasoline tax is increased above 1.23 R$l^{-1} and the hydrous ethanol is tax-free (see Chapter 5). In this case, the model also provides insights into what data need to be collected so as to reduce the uncertainty in the gasoline tax solution space. Based on these insights, we recommend to research the mapping between gasoline tax and decision making as to ethanol production.

These case studies illustrate that actors' behavior drive system behavior. Patterns in production and production capacity of biofuels hinge on actors' decision making as to investment, production, and consumption of biofuels. This decision-making process is influenced by both formal institutions (e.g. policies such as taxes, blending mandates, and subsidies) and informal institutions (e.g. perceptions of the biofuel market and preferences in production and consumption of biofuels).

7.2.3. WHAT INSTITUTIONAL CONDITIONS ARE CONDUCIVE TO THE EMERGENCE OF A BIOJET FUEL SUPPLY CHAIN FROM AN EXISTING ROAD TRANSPORT BIOFUEL SUPPLY CHAIN?

We used the model developed in the study of the Brazilian sugarcane-ethanol supply chain for exploring the institutional conditions that might support the emergence of a biojet fuel supply chain. We limited our analysis to the production of biojet fuel from ethanol (alcohol to jet route) and to the effect of a feed-in tariff, capital investment subsidy, and gasoline tax on the emergence of the biofuel supply chain.

We found that the emergence of a biojet fuel supply chain from the existing Brazilian sugarcane-ethanol supply chain hinges on the interaction of the feed-in tariff and the gasoline tax. In a tax-free gasoline regime, a feed-in tariff above 3 R$l^{-1} stimulates the production of biojet fuel. Nevertheless, at higher levels of gasoline taxation (i.e. 2.46 R$l^{-1}), any feed-in tariff is insufficient to ensure the production of biojet fuel. This is due to that a high gasoline tax results in an increase in the demand for hydrous ethanol, which leads to an increase in its price. These conditions favors the production of hydrous ethanol. Thus, at these levels of taxation of gasoline it is necessary to introduce regulations on the production of biojet fuel to ensure its production. We also found that the influence of capital investment subsidy on the emergence of a biojet fuel supply chain is significant at high levels of gasoline tax. This is due to the constraints in the production of hydrous ethanol and biojet fuel imposed on the plants that benefit from the investment subsidy. At these levels of gasoline tax, it is the capital investment subsidy and its mandate as to the production of biojet fuel that sows the seed for the emergence of a biojet fuel supply chain and ensures a minimum in the biojet fuel production, respectively. Finally, we found that the feed-in tariff has the most significant contribution in the costs to spur biojet fuel production (see Chapter 6).

Since the Brazilian government aims to increase the consumption of hydrous ethanol in the road transport sector by 2030, the use of the existing sugarcane-ethanol sup-

ply chain as a platform for the emergence of a biojet fuel supply chain poses a policy dilemma as to the decarbonisation of the transport sector, if the alcohol to jet route was the only technology used to produce biojet fuel in Brazil. This dilemma is the trade-off between hydrous ethanol and biojet fuel production. One way out of this dilemma is to increase the level of gasoline taxation and to introduce regulations on the production of biojet fuel to ensure its production. We showed that under these institutional conditions, the production of biojet fuel is sufficient to satisfy the domestic demand of jet fuel in 2030 provided that this demand amounts to the 30% of the total demand. Nevertheless, given the international nature of aviation and that there is major local control over road transportation, it is expected that policies are designed and implemented to spur the production of biofuels in the road transport sector (see Chapter 6).

All things considered, while optimization/equilibrium models can provide insights into the evolution of a biofuel supply chain, these insights are provided from a normative viewpoint. That is, these models provide information about the "ideal" evolution of a biofuel supply chain from a technical, economic, or environmental perspective. To translate these ideal visions into specific policy portfolio, however, we need a model that aims to describe the relevant processes at work in the system. The models developed in this research may be used to assess whether certain policy measures could achieve the desired state described by the optimization/equilibrium models.

7.3. REFLECTION

IN this section, we will reflect on the scientific contribution of this study and the conceptual framework and models developed in this research.

7.3.1. SCIENTIFIC CONTRIBUTION

Starting the reflection, we position this research within the grander scheme of science. This works fits within the domains of (energy) policy analysis and energy system analysis and modeling. In the domain of (energy) policy analysis, where formal analysis has neglected the effect of social processes and social structures on the evolution of energy systems, this study describes both how to incorporate social processes and social structures into the analysis and what is the effect of these processes and structures on the evolution of the system. In the domain of energy system analysis and modeling, this study provides the conceptual and analytical tools to gain more insights into the processes and mechanisms at work in the energy systems.

The main scientific contributions of this research are the following:

- Framework: the conceptual framework developed in this research offers an alternative for thinking about biofuel supply chains and describing agent-based models. Concepts from the **M**odeling **A**gent system based on **I**nstitutional **A**nalysis (MAIA) framework and from the **O**verview, **D**esign concepts, and **D**etails (ODD) protocol are used along with the conceptual framework to describe the agent-based models.

- Methodological improvements in the agent-based modeling of biofuel supply chains: in this study, we illustrate how the conceptual framework grounds the modeling of

social structures (e.g. spot markets and contracts), policies (e.g. taxes, subsidies, blending mandates, and feed-in tariffs), and actors behavior (e.g. decision making about production and consumption of biofuels)

- Insights into the workings of existing biofuel supply chains: in this study, we provide insights into the effect of policy instruments and actors' behavioral mechanisms on the evolution of biofuel supply chains.

The conceptual framework developed in this study, the methodological improvements in the modeling of biofuel supply chains, and the insights into the workings of existing biofuel supply chains may contribute to the transition towards to a sustainable energy system by assisting in the design of more efficient policy instruments that aim to spur the production and consumption of biofuels.

7.3.2. CONCEPTUAL FRAMEWORK

The conceptual framework developed in this dissertation offers an alternative for thinking about biofuel supply chains and describing agent-based models. The framework enables us to incorporate social structures and social processes in the design of the agent-based model. Furthermore, the scope of the framework can be extended to the analysis of other socio-technical systems such as energy systems, water systems, and mobility infrastructure.

Two concrete advantages of the conceptual framework are exploited when this is formalized into an agent-based model. Firstly, the computational model offered a test bed for hypotheses of system behavior. For instance, in the analysis of the German biodiesel supply chain (see Chapter 3), we found that the patterns observed in the actual development of production and production capacity can, to a certain extent, be explained by investors' optimistic perceptions of the market development.

Secondly, the computational model facilitated the systematic exploration of the effect of policies and actors' behavior on the evolution of the system. This exploration provided insights that might underpin the future policy making to foster the emergence of new biofuel supply chains. For instance, in the analysis of the German biodiesel supply chain (see Chapter 4), we found that actors' adaptation mechanisms to changes in price heavily influence the production of biodiesel. In the analysis of the Brazilian sugarcane-ethanol supply chain (see Chapter 5), we found that an increase in the gasoline tax above $1.23\,\mathrm{R\$l^{-1}}$ leads to double the production of ethanol by 2030. Finally, in exploring the emergence of a Brazilian biojet fuel supply chain (see Chapter 6), we found that, if the alcohol to jet route was the only technology used to produce biojet fuel in Brazil, either a tax-free gasoline regime and a feed-in tariff of $6\,\mathrm{R\$l^{-1}}$ or a high level of gasoline taxation and the introduction of mandates in the production of biojet fuel, lead to the emergence of a biojet fuel supply chain.

One of the main limitations of the conceptual framework is to neglect the effect of ecological elements on the behavior of the system. Socio-technical systems are unable to function without the services provided by natural ecosystems (i.e. provision of food, water, and resources, control of climate, decomposition of wastes). If the framework is to be used to analyze the impact of socio-technical systems on the environment (e.g. climate change, deforestation, pollution) and vice versa, the relationships and feedbacks

among ecosystem, social, and physical processes need to be incorporated into the conceptual framework.

7.3.3. AGENT-BASED MODELS OF BIOFUEL SUPPLY CHAINS

In this study, we developed empirically-grounded agent-based models as the biofuel supply chains analyzed in this research are site and context-specific. These models incorporate both governance structures and the effect of actors' preferences and policies on actors' behavior. The agent-based models were designed to provide insights into the processes at work in the evolution of biofuel supply chains.

In this research, through the different case studies, we developed six methodological improvements with respect to the traditional approach in the (agent-based) modelling of biofuel supply chains. In the modelling of the German biodiesel supply chain, we described (i) how the conceptual framework underpinned the conceptualization of a biofuel supply chain, (ii) how the conceptual framework enabled the incorporation of social structures such as the spot market, social processes such as competition for feedstock, and actors' behavior such as decision making about land use into the design of the agent-based model, and (iii) how the MAIA framework can be used to operationalize formal institutions such as blending mandates, taxes, and subsidies (see Chapter 3). In the modelling of the Brazilian sugarcane-ethanol supply chain, we described (iv) how to introduce the spatial dimension into the modelling of biofuel supply chains as decision making about investments in processing capacity hinges on location and availability of the land to produce the feedstock, and (v) how to model both social structures such as contracts and actors' behavior such as decision making about production and consumption of ethanol (see Chapter 5). In the modelling of the emergence of a Brazilian biojet fuel supply chain, we described (vi) how to model formal policies such as feed-in tariff and capital investment subsidies (see Chapter 6).

The models developed in this research enable one to explore and clarify the effect of institutions and actors' behavior on the behavior of biofuel supply chains. For instance, the model developed to analyze the German biodiesel supply chain can be used to understand how actors' behavioral mechanisms, the timing of government interventions, and interaction of agricultural and bioenergy policies shape patterns in production and production capacity of biodiesel (see Chapter 3 – Chapter 4). The model developed to analyze the Brazilian sugarcane-ethanol supply chain can be used to provide insights into what institutional conditions lead to an increase in the production of hydrous ethanol (see Chapter 5). Finally, the model of the sugarcane-ethanol supply chain in Brazil can be used to explore what institutional conditions are conducive to the emergence of a biojet fuel supply chain (see Chapter 6).

Nonetheless, the models developed in this research have several limitations. First, the generalization of the outcomes of the models is limited because the models were designed to account for the essential processes and structures relevant to the modeling problem, which is site and context-specific. Second, the models neglect the effect of institutions on organizational structures. Third, as it is impossible for one model to capture all of the complexity of socio-technical systems, the outcomes of the models hinge on the developments of several exogenous parameters. Finally, the models exclude the effect of non-economic attributes such as trust, peer pressure, and values on actors' de-

cision making.

7.3.4. BIOFUEL SUPPLY CHAINS EVOLUTION

Brazil and Germany provide contrasting pictures of biofuel supply chains in the world in terms of structure and natural resources. From the structural viewpoint, the Brazilian sugarcane-ethanol supply chain is more complex than the German biodiesel supply chain. The Brazilian biofuel supply chain is characterized by its flexibility in the production, where sugar and ethanol compete for the same feedstock (sugarcane), and by two competing demands for ethanol, whereas the German biodiesel supply chain is less flexible in both production and consumption of biodiesel. These differences in structure emerge from the co-evolution of biofuel supply chain's structure with actors' behavior, national policy interventions, natural resources, and global market forces.

Two policy interventions played an important role in the emergence of the German biodiesel supply chain. The set-aside premiums of the EU Common Agricultural Policy and the tax exemption for biodiesel. The set-aside premiums provided the incentives for growing non-food crops. The tax exemption ensured that biofuels are price competitive as consumers in Germany only purchase biodiesel if it is price competitive with diesel. These two policy interventions plus the positive actors' perception of the biofuel market accelerated the expansion of the biofuel sector in Germany.

The gasoline tax will be one of the main drivers of the future expansion of the sugarcane-ethanol supply chain in Brazil. This policy intervention was already used in the past to consolidate the ethanol agro-industry. Nevertheless, the government needs to be cautious when implementing this policy as it can have negative impacts on the productivity level of ethanol producers or in the ethanol prices. The gasoline tax may disincentive ethanol producers in striving for technological improvements as this protection mechanism guarantee that ethanol is competitive with gasoline.

These case studies shed light on how policy interventions may shape the evolution of biofuel supply chains. From the analysis of the German biodiesel supply chain, we learnt that a nascent biofuel supply chain needs to be nurtured and protected from a competitive environment to ensure its development. From the analysis of the Brazilian sugarcane-ethanol supply chain, we learnt that the creation of an institutional framework that internalizes the external costs of fossil fuel production is a promising mechanism to consolidate a biofuel industry. Unfortunately, extrapolating these lessons to biofuel supply chains in other countries is not straightforward. The success of policy interventions in another country hinges on the interaction of the country's social context, institutional framework, infrastructure, and natural resources.

7.4. LESSONS LEARNT

THE goal of this research was to contribute to enhance our understanding of the emergence of biofuel supply chains. In addition, we aimed to provide insights into the workings of successful biofuel supply chains such as the German biodiesel supply chain and the Brazilian sugarcane-ethanol supply chain.

We approached this goal by developing a conceptual framework that incorporates both the technical and the social elements of a biofuel supply chain and the institutional

conditions governing their behavior. To explore the processes at work in the evolution of biofuel supply chains, we formalized the conceptual framework into an agent-based model.

The conceptual framework is compatible with economic theory, rational choice theory, transaction cost theory, and theory of planned behavior. In this research, however, we use largely the rational choice theory to describe actors' behavior. This theory adequately describes biofuel producers' behavior and, to a certain extent, (bio)fuels consumers and farmers' behavior. Alternatively, theories that account for institutional factors in the decision making or data-driven decision-making models (e.g. econometric models, machine learning models) may be used to represent farmers' behavior.

We show that the conceptual framework offers a systematic method to identify social processes and structures that underlie the agent-based model's design. That is, the conceptual framework identifies the elements that one needs to consider for the modelling of a biofuel supply chain such as: actors' decision making and interaction, social structures, and the effect of policies on actors' behaviour. This is considered useful in the light that current biomass/biofuels markets models neglect the effect of social processes and social structures on the evolution of the system. As we showed in this research, these processes play an important role in the evolution of a biofuel supply chain.

Nevertheless, the formalization of the framework into an agent-based model is an ambiguous process. This process intertwines art and science. The art of modeling involves the articulation and the translation of the knowledge of domain experts and stakeholders into a conceptual model, while keeping this abstraction simple yet useful. The science of modelling involves the translation of the abstract concepts to mathematical/computational language. As we show through the case studies (see Chapter 3 – Chapter 6), the **M**odelling **A**gent systems using **I**nstitutional **A**nalysis (MAIA) framework and the **O**verview, **D**esign concepts, and **D**etails (ODD) protocol proved to be useful in reducing the ambiguity of the modelling process.

One of the challenges in the development of an agent-based model is its parameterization because of the lack of or poor quality data. Nevertheless, lack of data should never be used to decide whether certain processes or mechanisms need to be modeled or not. Instead, lack of data should be used to inform future data collection. For instance, in the modeling of the Brazilian ethanol supply chain, we recommend mapping the relationship between gasoline tax and decision making as to ethanol production so as to improve the heuristics used to model the decision making of biofuel producers.

Computational models are being increasingly used to inform public policy making. The common assumption is to use these models to make predictions despite that our understanding of systems that involves social and economic phenomena is still quite limited. This assumption has led both to emphasize the role of the model validation step in the development of models and to focus on the model results. From a Popperian viewpoint, a model cannot be validated as the model is a formalization of a theory, and a theory cannot be validated but falsified. On the other hand, it is impossible to develop models that make an accurate prediction of the state of socio-technical systems as these systems are not isolated in the real world. That is, there may be unexpected exogenous factors that affect the model outcomes and that are neglected in the model conceptualization. Therefore, rather than focusing on the model validation step and model out-

comes and their accuracy, (i) problem-owner(s), stakeholder(s), and modeler(s) should pay more attention to the processes of model development and use, and (ii) the models should be used to formalize and provide insights into the processes at work in the respective domain.

The exercise of modeling to inform policy making requires careful consideration of ethical issues. Some such considerations are the degree of uncertainty present in the results derived from the model and the assumptions that underpin the model structure. Modelers should clearly communicate both the degree of uncertainty present in the results derived from the model and the model assumptions. Above all, modelers should inform about the implications of that parametric and structural uncertainty in the policymaking.

The models developed in this research capture a contextual truth as the conclusions derived from these models apply to a specific setting. Hence, the policymakers should be cautious if the insights provided by this research are to be used to underpin the design and evaluation of biofuel policies elsewhere. Indeed, we recommend to policymakers, if possible, to opt for an eclectic approach in the analysis of policies to incentivize the creation of new biofuel policies. That is, we encourage policymakers to base their conclusions on the insights provided by models with different assumptions about the mechanisms and processes that bring about system behavior.

Yet, this research is a step forward in the development of models that provide a richer description of biofuel supply chains. First, the agent-based models developed in this research illustrate how to incorporate the effect of actors' preferences in their decision making, how to include governance structures, and how to map biofuel policies onto actor behavior. Notwithstanding their importance, these elements are neglected by mainstream approaches. Second, the approach proposed in this study could be used in three different manners: (i) it can be used as a means to explore different mechanisms that lead to the equilibrium predicted by the studies based on optimization and neo-classical economics, (ii) it can be used to explore whether this equilibrium might be reached, and (iii), as it is impossible to capture all of the complexity of socio-technical systems in one single model, the agent-based models developed with this approach could be coupled with models built to describe either biomass/biofuels markets or relevant phenomena (e.g. land use change) in different geographies. Thereby, we can account for the effect of global market forces on the evolution of biofuel supply chains. In short, this approach could be used to provide insights into the effect of different future deployment strategies on bioenergy systems development.

Finally, we argue that the incorporation of the influence of institutions on the performance of bioenergy systems should be a fundamental part of the research agenda. As we showed through the different case studies (see Chapter 3 – Chapter 6), institutions influence behavior, which in turn determines the properties of the system. In addition, given that biofuel supply chains are complex and context-dependent, we argue that we should strive for both developing models that incorporate the necessary causal mechanisms for a reliable description of the problem at hand and, if necessary, integrating models that describe biomass/biofuel markets in different geographies. The multimodel ecology[3]

[3] Multimodel ecology is defined as *"an interacting group of models coevolving with one another in a dynamic sociotechnical environment"* [232]

approach may be useful to facilitate model integration. The richness of socio-technical systems cannot be compressed into unique modeling paradigms.

7.5. FURTHER RESEARCH

IN this final section, we propose several areas for future work.

Extending the agent-based model of the Brazilian sugarcane-ethanol supply chain: in the analysis of the effect of policy instruments (i.e. blending mandates and taxes levied on gasoline, hydrous, and anhydrous ethanol) on the production and consumption of hydrous and anhydrous ethanol (see Chapter 5), we assume that the adoption of flex vehicles and regular vehicles was exogenous. In reality, this adoption may depend as well on developments of prices for gasohol and hydrous ethanol. Thus, we recommend introducing the adoption of vehicles within the scope of the model. The **T**echnology **A**cceptance **M**odel (TAM), which models the process whereby users come to accept and a use a technology, may be used to guide the conceptualization of the adoption of either flex or regular vehicles in the Brazilian context.

Integration of agent-based models with other modeling paradigms: the inherently international nature of the aviation sector poses a serious challenge in the analysis of the evolution of biojet fuel supply chains. To provide a better description of this phenomenon, it is necessary to account for the interaction of biomass/biofuels markets at the national and international level as well as the developments of global market forces. As it is impossible to capture all of the complexity of socio-technical systems in one single model, we recommend further research into the integration of models (e.g. agent-based models, optimization models, general/partial equilibrium models) that describe biomass/biofuel markets in different geographies to provide insights into how biojet fuel supply chains may evolve. The multimodel ecology approach may be useful to facilitate model integration. This combination of different modeling paradigms can be also used to provide more refined insights into how transitions in energy systems, agricultural systems, and infrastructures can take place and how they could be effectively incentivized.

Exploring the co-evolution of institutions and (bio)energy systems: in this research, we focus on the emergence or evolution of biofuel supply chains rather than the emergence of institutions necessary to create and develop those biofuel supply chains. In reality, institutions co-evolve with the (bio)energy system. Thus, from the theoretical viewpoint, we recommend further research into the co-evolution between institutions and system behavior. The modeling of this phenomenon is a crucial next step. This avenue of research might provide insights into what conditions lead to institutional change and how this change influences the behavior of the system. The method proposed in this study along with machine learning techniques can be used for this exploration. Machine learning techniques enable finding patterns and to learn based on input data. An alternative to model the emergence of institutions is by incorporating the policymaker into the scope of the model. Machine learning techniques can be used to model the policymaker's learning processes necessary for the design and evaluation of new policy instruments.

Exploring system behavior under deep uncertainty: the method proposed in this work can be coupled with the **E**xploratory **M**odelling and **A**nalysis method (EMA)[4] to provide insights, given a variety of uncertainties, into the different operating regimes of the phenomenon under study. In addition, this coupled method can be used as an analytical tool to assist in the design of more robust policy instruments.

Accounting for non-economic attributes in the decision-making models: by large, the institutions analyzed in this research are focused on fiscal policies. We neglected the effect of non-economic attributes such as trust, peer pressure, and values on actors' decision making. The models of actors' decision making used in this research can be improved by using machine learning techniques, or econometric models. Any improvement in the predictive power of the decision-making process, however, comes at a cost. It clouds the understanding of the underlying mechanism of the process. Therefore, it is up to the modeler to assess the trade-off between prediction and transparency based on the purpose of the model.

[4] See S. Bankes, Exploratory modeling for policy analysis, Oper. Res. 4 (1993) 435–449.

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[232] Bollinger L. Andrew, Nikolić Igor, Davis Chris B., and Dijkema Gerard PJ. Multimodel ecologies: Cultivating model ecosystems in industrial ecology. *Journal of Industrial Ecology*, 19(2):252–263. doi:10.1111/jiec.12253. URL https://onlinelibrary.wiley.com/doi/abs/10.1111/jiec.12253.

[233] Sujith Nair and Hanna Paulose. Emergence of green business models: The case of algae biofuel for aviation. *Energy Policy*, 65:175 – 184, 2014. ISSN 0301-4215. doi:https://doi.org/10.1016/j.enpol.2013.10.034. URL http://www.sciencedirect.com/science/article/pii/S0301421513010562.

Appendices

A

GERMAN BIODIESEL SUPPLY CHAIN: AGENTS DECISION MAKING

A.1. FARMERS

A.1.1. ALLOCATION CROPS

The main farmers' decision making is about land use. The allocation decision making is influenced by the policy framework. When the agricultural reform is binding the allocation problem is restricted to the cultivation of rapeseed on the set-aside land. Figure A.1 presents the algorithm used for the decision making.

Profits are calculated with the following equations:

$$\pi_{r_i} = \left(\left(P_{r_i}^{exp} - c_{r_i}\right) q_{r_{unit}}\right) + \left(S_r q_{r_{unit}}\right) \tag{A.1}$$

$$\pi_{w_i} = \left(\left(P_{w_i}^{exp} - c_{w_i}\right) q_{w_{unit}}\right) + \left(S_w q_{w_{unit}}\right) \tag{A.2}$$

where:
π: profits generated by cultivating the crops per square meter, €m^{-2}
P^{exp}: expected price, €t^{-1}
c: production cost, €t^{-1}
q_{unit}: mass of crop per square meter, tm^{-2}
S: subsidies, €t^{-1}
i: ID of the farmer
r: rapeseed
w: wheat

As shown in Figure A.1 the algorithm starts with the calculation of the profits per area. Then, stocks for rapeseed are checked. If the current profits are positive the farmer will grow rapeseed in the set aside land. Otherwise, he will not grow rapeseed. Stocks define how much rapeseed to cultivate in the set aside land. If all the rapeseed was sold

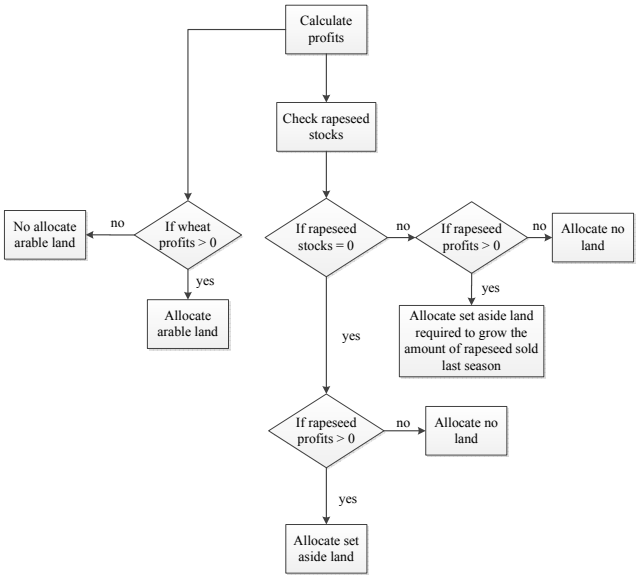

Figure A.1: Algorithm used for farmers to allocate land when the agricultural reform is binding

last season (stocks = 0) farmer will use all of the set aside land available. Otherwise, he will only use the land required to produce the same amount of rapeseed sold last season. The allocation of land to cultivate wheat is assumed to be only a function of profits. The decision making was designed to incorporate the concepts of imperfect information and feedback mechanisms. Profits are calculated based on (endogenous) expectations for rapeseed and wheat prices. The allocation of land is not only a function of economic indicators but also of past performance. The information feedback is used to correct the allocation. When the liberalization of the market is binding the allocation problem involves a direct competition for arable land between rapeseed and wheat. Figure A.2 presents the algorithm used for the decision making.

Profits are calculated with the following equations:

$$\pi_{r_i} = \left(\left(P_{r_i}^{exp} - c_{r_i}\right) q_{r_{unit}}\right) + \left(\left(S + eS\right)\left(\frac{q_{r_{unit}}}{Y_{r_i}}\right)\right) \tag{A.3}$$

$$\pi_{w_i} = \left(\left(P_{w_i}^{exp} - c_{w_i}\right) q_{w_{unit}}\right) + \left(S\left(\frac{q_{w_{unit}}}{Y_{w_i}}\right)\right) \tag{A.4}$$

where:
π: profits generated by cultivating the crops per square meter, €m^{-2}
P^{exp}: expected price, €t^{-1}
c: production cost, €t^{-1}

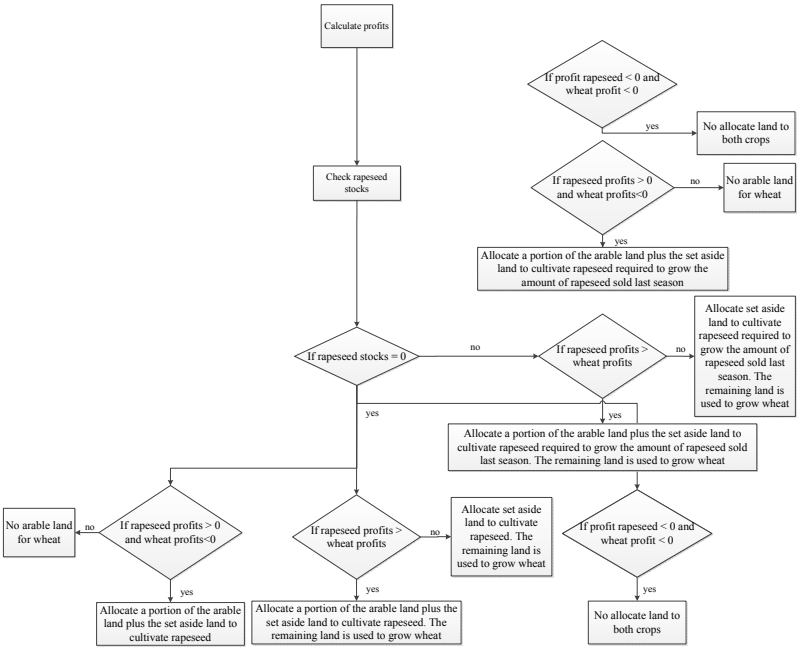

Figure A.2: Algorithm used for farmers to allocate land when the liberalization of the agricultural market is binding

q_{unit}: mass of crop per square meter, $\mathrm{t\,m^{-2}}$
S: standard agricultural subsidy, $€\,\mathrm{ha^{-1}}$
eS: extra fee for energy crops, $€\,\mathrm{ha^{-1}}$
Y_r: yield of rapeseed, $\mathrm{t\,ha^{-1}}$
Y_w: yield of wheat, $\mathrm{t\,ha^{-1}}$
i: ID of the farmer
r: rapeseed
w: wheat

The algorithm presented in Figure A.2, although shares the same characteristics and logic of that presented in Figure A.1, it introduces the direct competition between rapeseed and wheat for land.

A.2. BIOFUEL PRODUCERS

A.2.1. PRODUCTION CAPACITY EXPANSION

Biofuel producers' decision making on capacity expansion is assumed to be influenced by the following factors:

- Feedstock supply.

- Biodiesel demand.
- Profitability measures (NPV).
- Perception on both agricultural and bioenergy markets' development.

As shown in Figure A.3, biofuel producers first check the availability of rapeseed and their biodiesel stocks. If they find out that there is enough rapeseed supply to operate the plant and that the biodiesel produced have been sold they will consider invest on new capacity. A profitability analysis (NPV) will determine the feasibility of the project. If NPV is positive the biofuel producer will invest on new capacity. The number of plants to be built is based on the producer's perception of biomass and/or bioenergy markets developments.

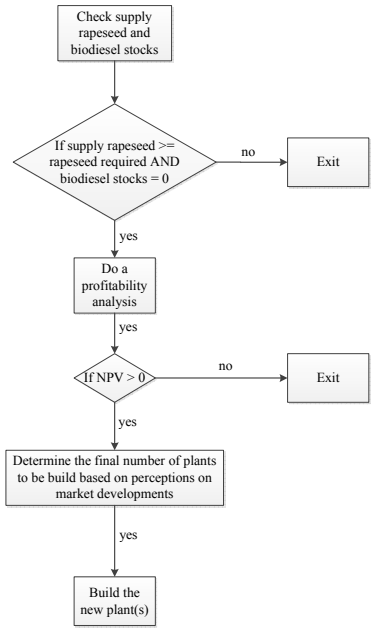

Figure A.3: Algorithm used for biofuel producers to determine the number of plants to be built

B

TECHNO-ECONOMIC DATA OF THE PRODUCTION OF BIODIESEL IN GERMANY

Table B.1 shows the capital expenditure (CAPEX) used in the study. The data was obtained from Charles et al.[1] It was assumed that the CAPEX is a step function of capacity. The total depreciable capital and the working capital were assumed to be 80% and 20% of CAPEX, respectively.

Table B.1: Estimates of capital expenditure costs

Capacity [$t yr^{-1}$]	CAPEX [$€ l^{-1}$]
8000	0.11
8000-30000	0.09
30000-100000	0.08

Production and financing assumptions are presented in Table B.2. A 0.7:0.3 debt-to-equity ratio was assumed. The corporate tax rate was assumed to be the biodiesel tax ($0.3 € l^{-1}$). The plant start-up is presented in Table B.3.

[1] Charles, C., et al., Biofuels—At What Cost? A review of costs and benefits of EU biofuel policies. 2013, Global Subsidies Initiative: Geneva.

Table B.2: Financing and production assumptions

Parameter	Value	Unit
Plant lifetime	25	yr
Depreciation period	10	yr
Rate of principal payments	10	yr
Debt: equity ratio	70/30	–
Interest rate on debt	8	%
Corporate Tax rate	0.3	[€l^{-1}]
Discount rate	10	%
Depreciation schedule	Straight line	–
Capacity factor	90	%

Table B.3: Plant start-up schedule

Year	TCI schedule	Plant availability
-2	33.3% Fixed Capital	0
-1	33.3% Fixed Capital	0
0	33.3% Fixed Capital	0
1		45%
2		67.50%
3		90%

C

YIELDS FOR RAPESEED AND WHEAT

Table C.1 presents the yields for rapeseed and wheat used in the study. The data were retrieved form FAO[1].

Table C.1: Yields for rapeseed and wheat for the period 1991 - 2014

Year	Rapeseed Yield [$t\,ha^{-1}$]	Wheat Yield [$t\,ha^{-1}$]
1991	3.3	6.77
1992	2.61	5.98
1993	2.83	6.58
1994	2.74	6.76
1995	3.19	6.89
1996	2.31	7.29
1997	3.14	7.27
1998	3.36	7.2
1999	3.58	7.54
2000	3.33	7.28
2001	3.66	7.88
2002	2.97	6.91
2003	2.87	6.5
2004	4.11	8.17
2005	3.76	7.47
2006	3.73	7.2
2007	3.44	6.96
2008	3.76	8.09
2009	4.29	7.81
2010	3.9	7.31

[1] FAO, FAOSTAT. Food and Agriculture Organization of the United Nations. Statistics Division.

Table C.1: Yields for rapeseed and wheat for the period 1991 - 2014

Year	Rapeseed Yield [$t\,ha^{-1}$]	Wheat Yield [$t\,ha^{-1}$]
2011	2.91	7.02
2012	3.69	7.33
2013	3.95	8
2014	4.48	8.63

D

BRAZILIAN ETHANOL SUPPLY CHAIN: MODEL CALIBRATION

This appendix describes the method used to estimate the parameters with high uncertainty in the model. It also presents the results obtained from the model calibration, and discusses the fit between historical data and model outcomes.

Some of the sources of high uncertainty in the model are the preferences in production of sugar and ethanol as well as preferences in the consumption of fuel. We incorporate the preferences in production of sugar and ethanol into the model by using the parameters: *minimum production ratio of sugar to ethanol and maximum production ratio of hydrous ethanol to anhydrous ethanol.* The minimum production ratio of sugar establishes the lower limit in the production of sugar compared to ethanol. This limit cannot be lower than the technical constraint (i.e 35%). The maximum production of hydrous ethanol establishes the maximum production of hydrous ethanol compared to anhydrous ethanol. Similarly, we incorporate preferences in consumption of E100 (hydrous ethanol) compared to gasohol (blend of gasoline with anhydrous ethanol) into the model by using the parameter *preference in the relative price of ethanol to gasohol.*

These preferences in production of ethanol and sugar as well as in consumption of ethanol vary among individual actors. To account for this heterogeneity in the preferences, we distributed these preferences among actors by assuming either a uniform or normal distribution. The parameters used to model these distributions were estimated based on historical data.

The approach used for the model calibration was *best-fit* calibration[1]. The model was calibrated for the period 2013-2016. The mean squared error was used as a measure of model fit to the time series. The calibration criteria are presented in Table D.1.

The objective function to be minimized is:

[1] Railsback, S. and V. Grimm, Agent-based and individual-based modeling: A practical introduction. 2011: Princeton University Press.

Table D.1: Calibration criteria

Year	Production ratio [%]		Production ratio [%]		Consumption ratio [%]	
	Sugar	Ethanol	Hydrous	Anhydrous	Hydrous	Anhydrous
2013	45.2	54.8	55.64	44.36	54.79	45.21
2014	43.2	57	57.59	42.41	53.95	46.05
2015	40.6	59.4	61.43	38.57	62.03	37.97
2016	46.3	53.7	57.48	42.52	55.67	44.33

$$f = \sum_{1}^{3} MSE_i \tag{D.1}$$

$$MSE_i = \frac{1}{n} \sum_{1}^{n} \left(\hat{Y}_i - Y_i\right)^2 \tag{D.2}$$

Where f is the objective function to be minimized, and MSE_i is the mean squared error of them calibration criterion *i*. $\hat{Y}$ is the vector of n predictions, and Y is the vector of observed values. It was assumed that the policy landscape remains stable during the period 2013-2016. The values of the policy instruments used in the minimization of the objective function are reported in Table D.2.

Table D.2: Policy instruments

Policy instrument	Value	Units
Blend mandate	23	%
Tax levied on gasoline	1.23	R\$l^{-1}
Tax levied on hydrous ethanol	0.3	R\$l^{-1}
Tax levied on anhydrous ethanol	0.05	R\$l^{-1}

The results of the minimization of the objective function are presented in Figure D.1. It was found that the effect of the minimum production ratio of sugar to ethanol on the objective function was negligible. When the values in the relative price of ethanol to gasohol were greater than 0.6, the objective function displayed a clearer pattern. This pattern was characterized for both exhibiting a minimum value for the objective function and for being robust. Table D.3 reports the values that yield a minimum in the objective function.

A comparison between the model outcomes and historical data is presented in Figure D.2 and Figure D.4. These figures show the median and the 90% envelope of the results obtained from the agent-based model developed in this study. Model outcomes were distilled from simulations that used the values reported in Table D.2 and Table D.3. The simulations consisted of 1000 repetitions. The historical data used for the model calibration (reported by UNICA[2]) is also presented in the figures.

[2]UNICA. unicadata. 2017; Available from: http://www.unicadata.com.br/index.php?idioma=2.

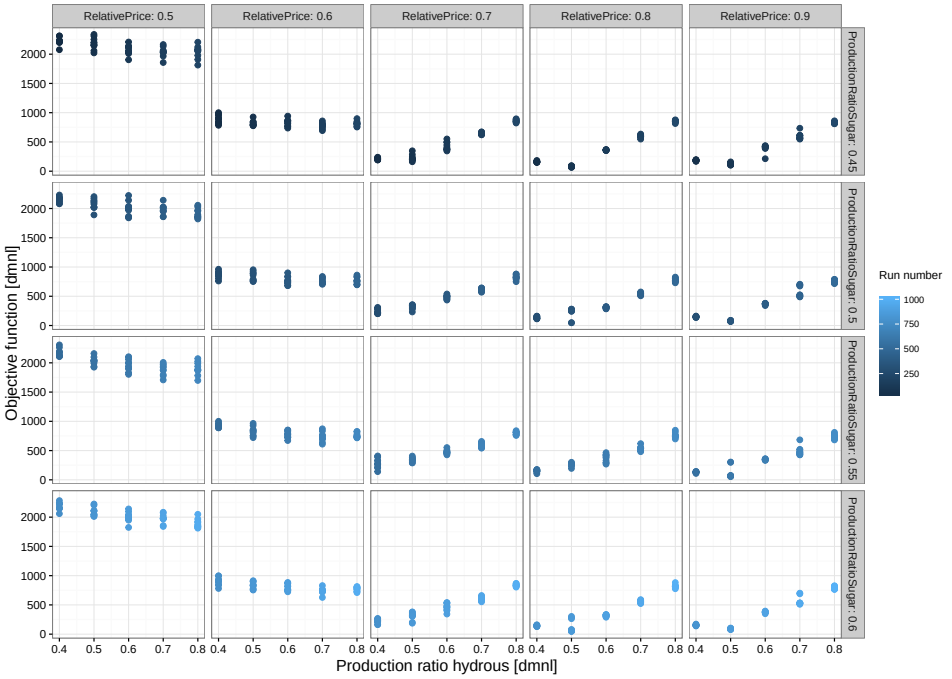

Figure D.1: Minimization of the objective function as a function of the mean of production ratio of hydrous, the mean of production ratio of sugar, and the mean in the drivers relative preference for relative price.

Table D.3: Results of the calibration

Parameter	Value
min production ratio sugar to ethanol[a]	0.5
max production ratio hydrous to anhydrous (in ethanol)[a]	0.5
preference in the relative price of ethanol to gasohol[b]	0.9

[a] the parameter calibrated is used to calculate the interval [a, b] of a uniform distribution.
$a = parameter - (parameter \cdot percentage - deviation)$;
$b = parameter + (parameter \cdot percentage - deviation)$.
The percentage of deviation is assumed to have a value of 10%.

[b] the parameter calibrated corresponds to the mean of a normal distribution. The standard deviation was assumed to have a value of 0.1. We use this value in the standard deviation to ensure that the distribution of the parameters lies on the specific interval in which the parameters have realistic values. From economic theory, these values lie around 0.7 (see Pacini and Silveira[3])

Model results for consumption ratio of hydrous to anhydrous ethanol were the calibration criterion that exhibited higher deviations with historical data (see Figure D.2).

[3] Pacini, H. and S. Silveira. Consumer choice between ethanol and gasoline: lessons from Brazil and Sweden. Energy Policy, 2011. 39(11): p. 6936-6942.

These deviations are because of the assumption of a stable policy landscape. Patterns in consumption ratio of hydrous to anhydrous ethanol are sensitive to the policy landscape, for the policies analyzed in this study aim to directly steer the drivers' consumption patterns.

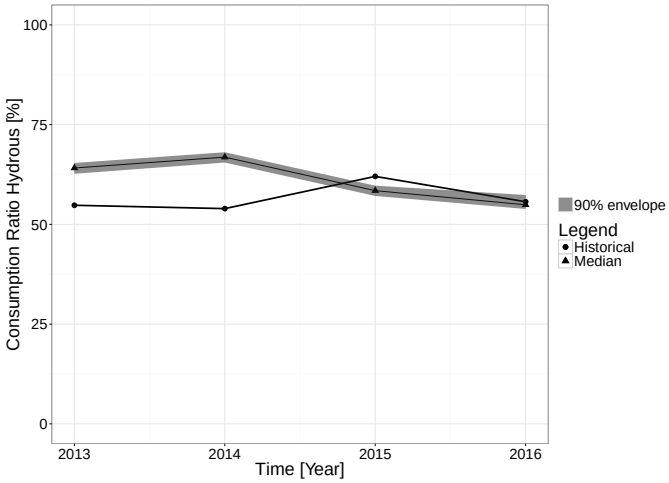

Figure D.2: Consumption ratio of hydrous to anhydrous ethanol over time: model results and historical developments. The confidence interval was calculated over 500 runs for the calibrated parameter values. Confidence interval: 90%

The higher difference between model outcomes and historical data for production ratio of hydrous ethanol to anhydrous ethanol occurred in the year 2015 (see Figure D.3). This discrepancy might be explained by the increase of the contribution for intervention in economic domain (CIDE) for gasoline in 2015[4]. This increase in the gasoline price led to higher demand for hydrous ethanol as consumers decisions are driven by the ratio between ethanol and gasoline prices in the pump. Major demand for hydrous ethanol led to an increase in the price of hydrous ethanol, and thus to a decrease in the production of anhydrous. This behavior was neglected by the model because of the assumption that policy instruments remain constant during the timeframe of the simulation. The agreement between the historical data and model outcomes for the production ratio of sugar to ethanol is high (see Figure D.4). With exception of the results related with the consumption ratio of hydrous to anhydrous ethanol, the model results exhibited a similar dynamic reported to that reported in the historical data.

[4] Barros, S. and C. Berk, Brazil. Biofuels Anual. Biofuels - Ethanol and Biodiesel, in GAIN report. 2015, USDA Foreign Agriculture Service.

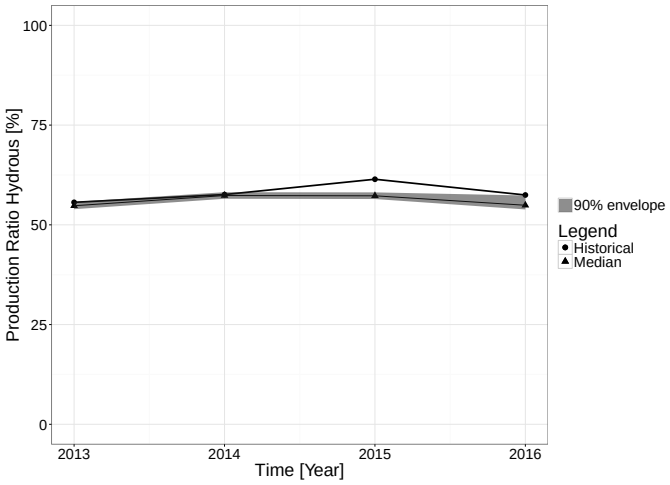

Figure D.3: Production ratio of hydrous to anhydrous ethanol over time: model results and historical developments. The confidence interval was calculated over 500 runs for the calibrated parameter values. Confidence interval: 90%

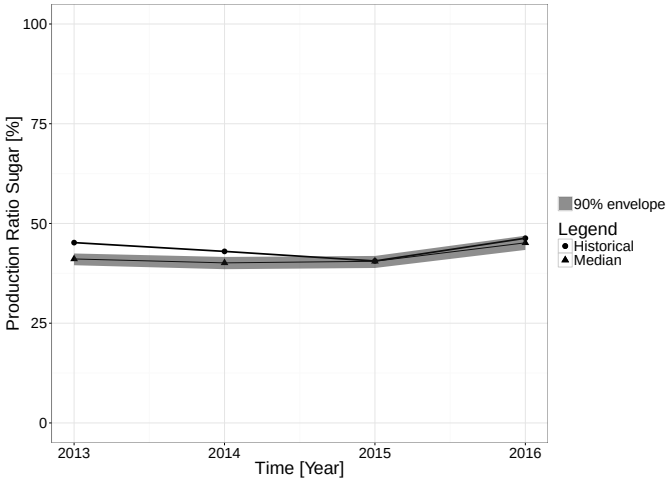

Figure D.4: Production ratio of sugar to ethanol over time: model results and historical developments. The confidence interval was calculated over 500 runs for the calibrated parameter values. Confidence interval: 90%

E

BRAZILIAN ETHANOL SUPPLY CHAIN: MODEL RESULTS

This appendix presents the results of the effect of fuel taxes and blend mandate on investment in production capacity, sugar and ethanol production, and ethanol demand. The results are presented in a matrix of 9 panels defined by the blend mandate and the gasoline tax variables. The effect of the hydrous tax is presented in each panel. For a given scenario of the tax levied on anhydrous ethanol, the 9 panels describe all of the possible permutations among blend mandate and taxes levied on gasoline and hydrous ethanol.

Figures below present the effect of anhydrous tax (i.e 0 and 0.1 Rl^{-1}, respectively) on the processing capacity (Figure E.1-Figure E.2), on consumption patterns of the owners of flex vehicles (Figure E.4-Figure E.5), and on the production of sugar (Figure E.6-Figure E.7) and ethanol (Figure E.8-Figure E.9). Figure E.3 presents spatial patterns in the deployment of new processing facilities for a simulation run other than one used in Figure 5.6.

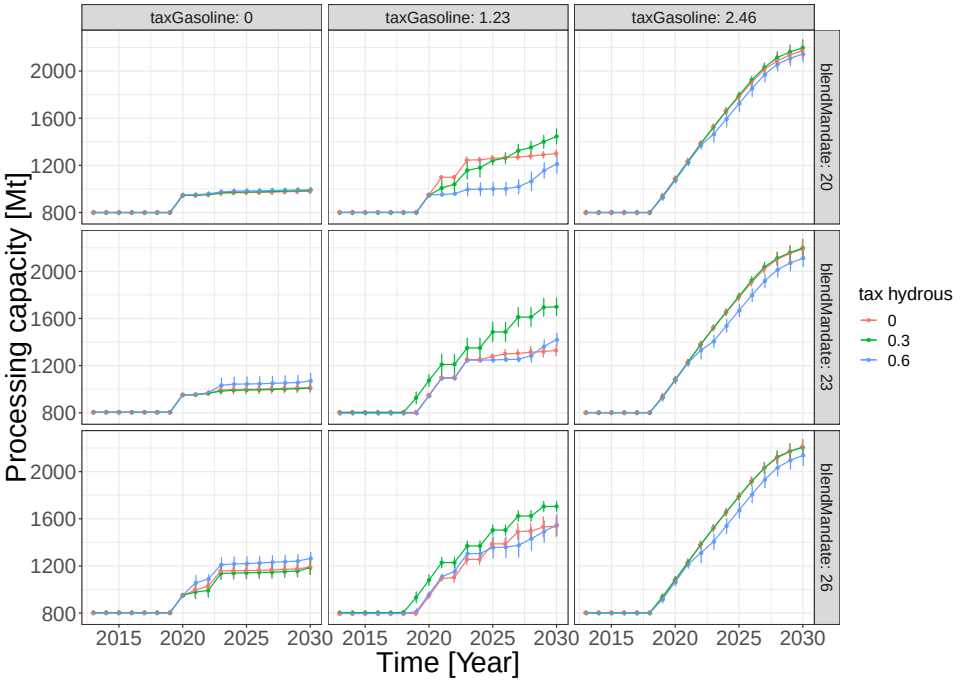

Figure E.1: Processing capacity of sugarcane as a function of time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R\$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0 R\$l^{-1}. Dots and the err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

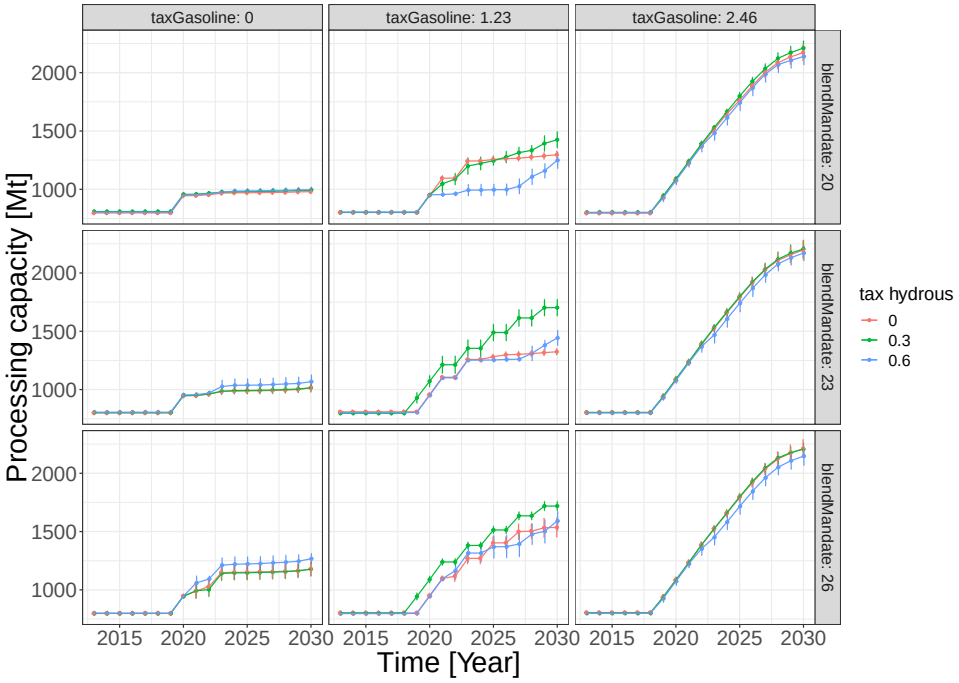

Figure E.2: Processing capacity of sugarcane as a function of time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R\$$1^{-1}$. Blend mandate in %v/v. Anhydrous tax = 0.1 R\$$1^{-1}$. Dots and the err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

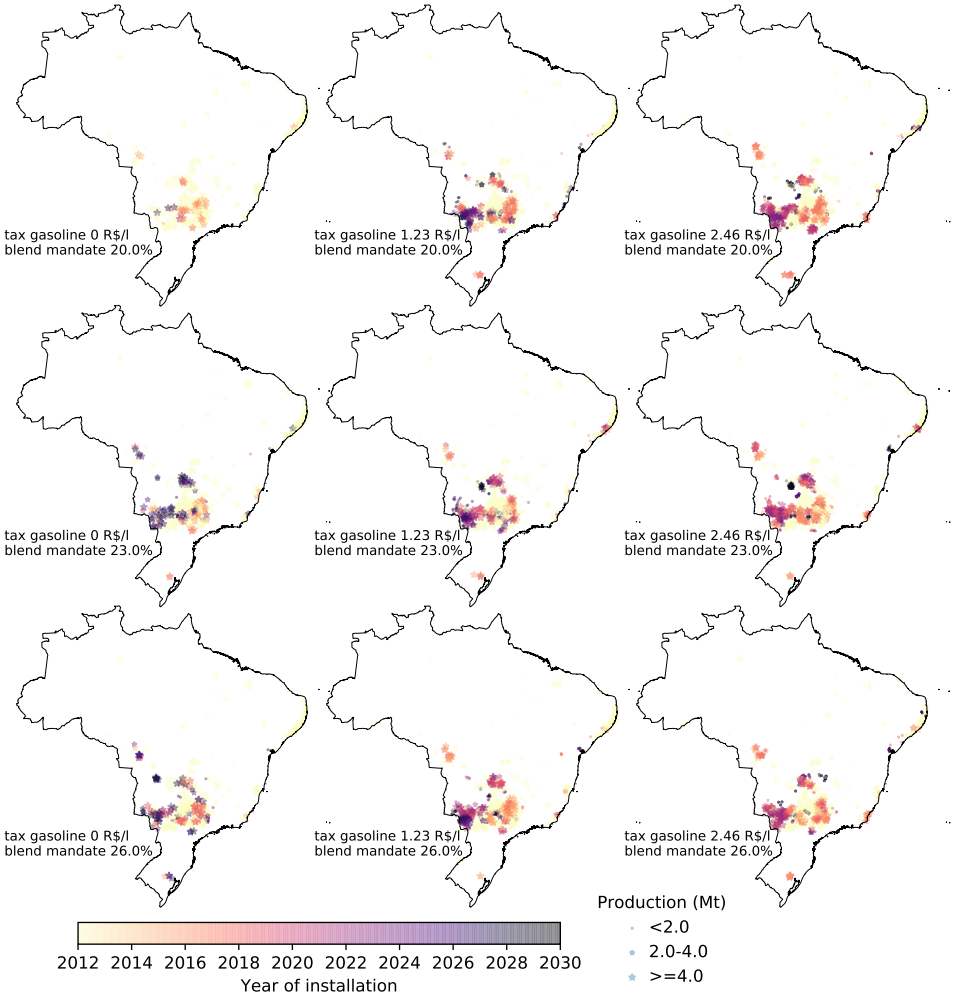

Figure E.3: Location, year of installation, and processing capacity of sugarcane plants as a function of different combinations of blend mandate and gasoline tax. Tax on gasoline in $R\$l^{-1}$. Blend mandate in %v/v. Hydrous tax = 0.3 $R\$l^{-1}$. Anhydrous tax = 0.05 $R\$l^{-1}$. This figure shows the results for a simulation run different to that used in Figure 5.6.

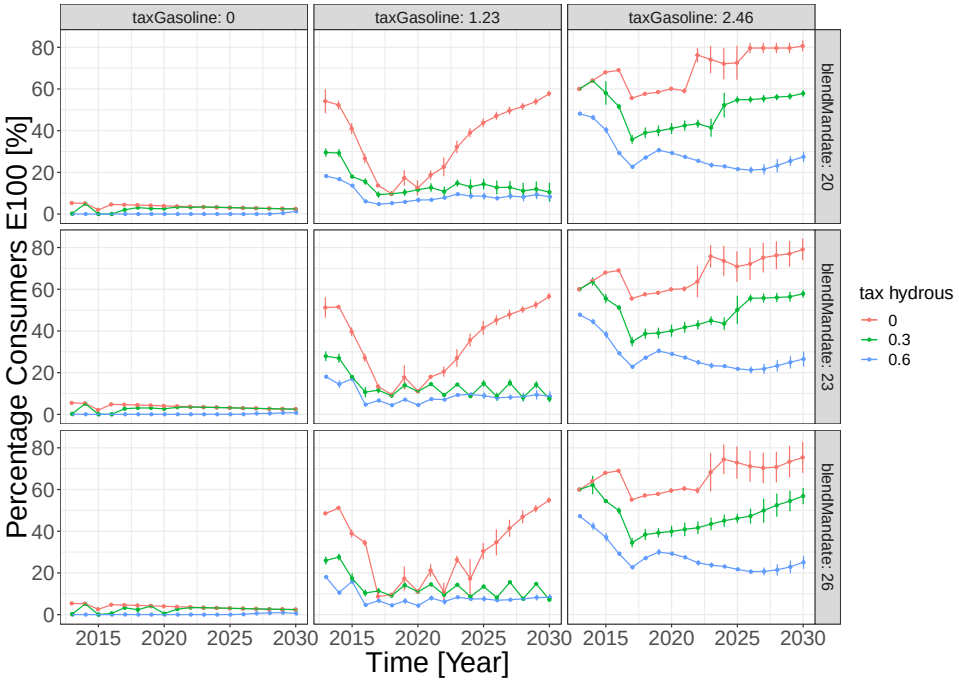

Figure E.4: Percentage of drivers that consume E100 over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in Rl^{-1}. Blend mandate in %v/v. Anhydrous tax = 0 Rl^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

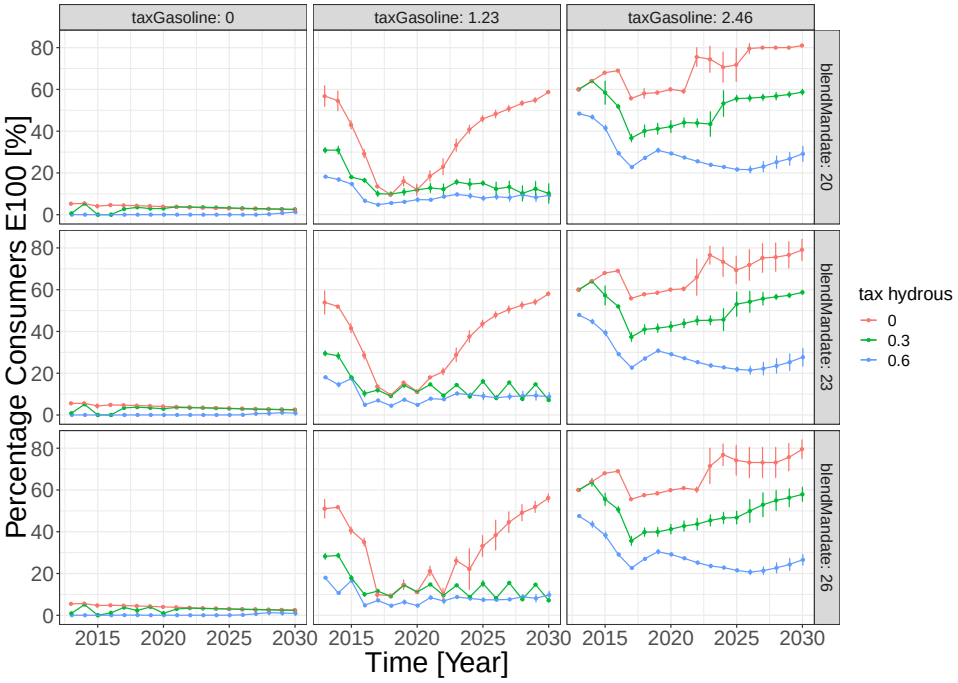

Figure E.5: Percentage of drivers that consume E100 over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.1 R$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

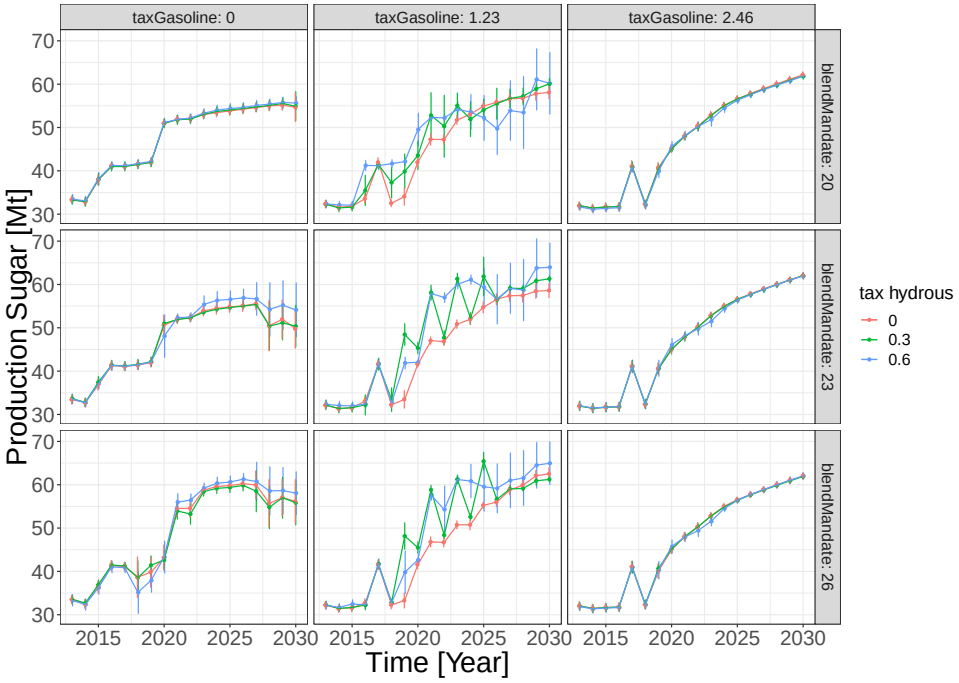

Figure E.6: Total production of sugar in Brazil over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R\$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0 R\$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

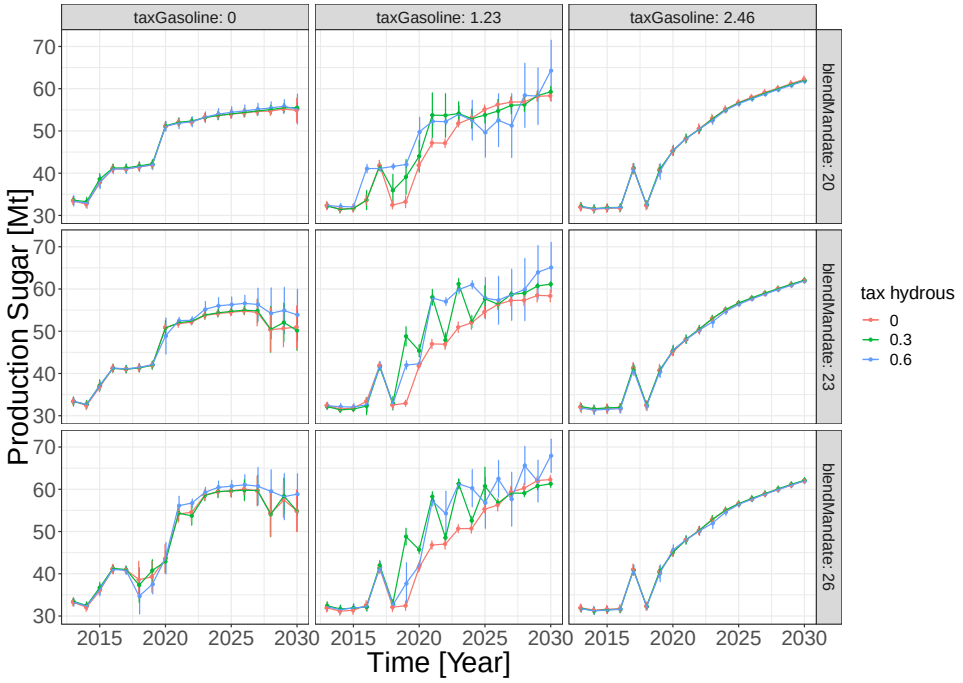

Figure E.7: Total production of sugar in Brazil over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in R$l^{-1}. Blend mandate in %v/v. Anhydrous tax = 0.1 R$l^{-1}. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

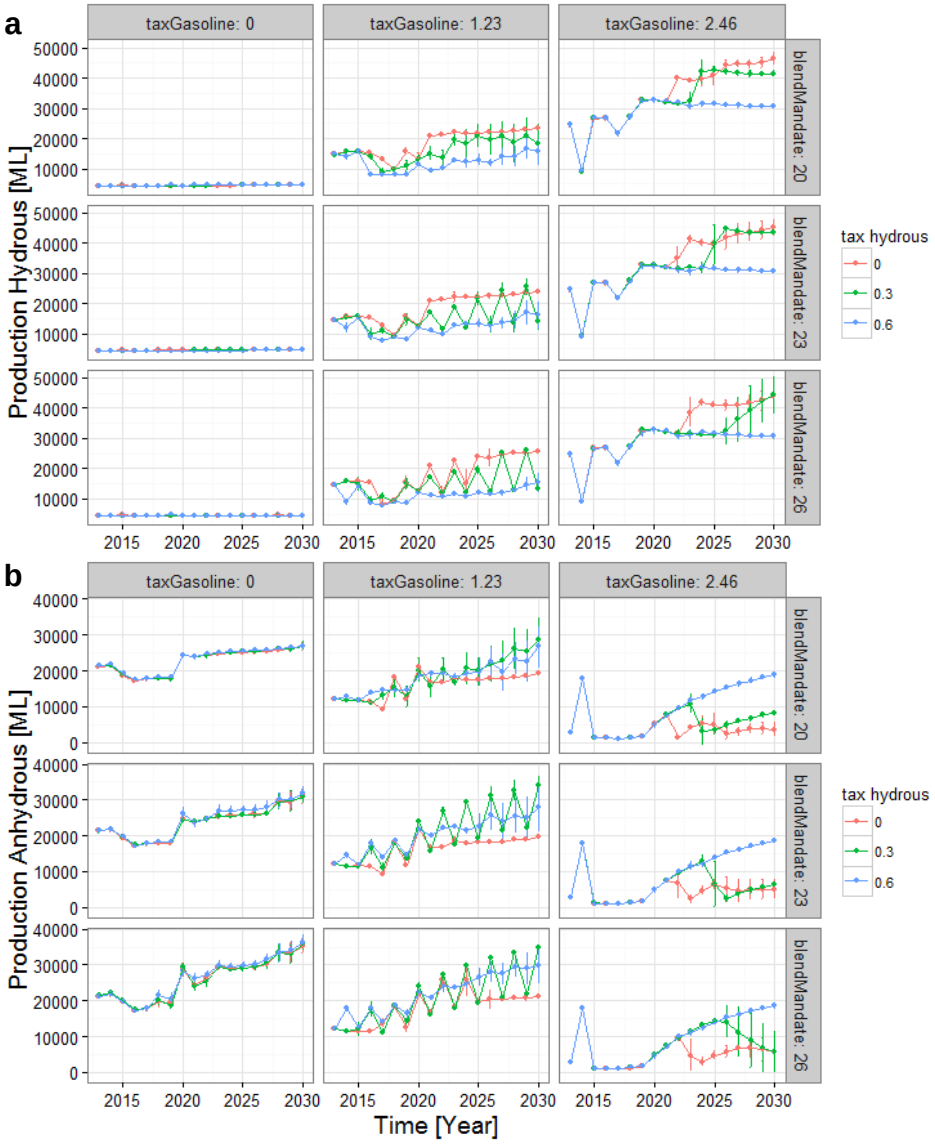

Figure E.8: Production of hydrous (**a**) and anhydrous ethanol (**b**) over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in $R\$l^{-1}$. Blend mandate in %v/v. Anhydrous tax = 0 $R\$l^{-1}$. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

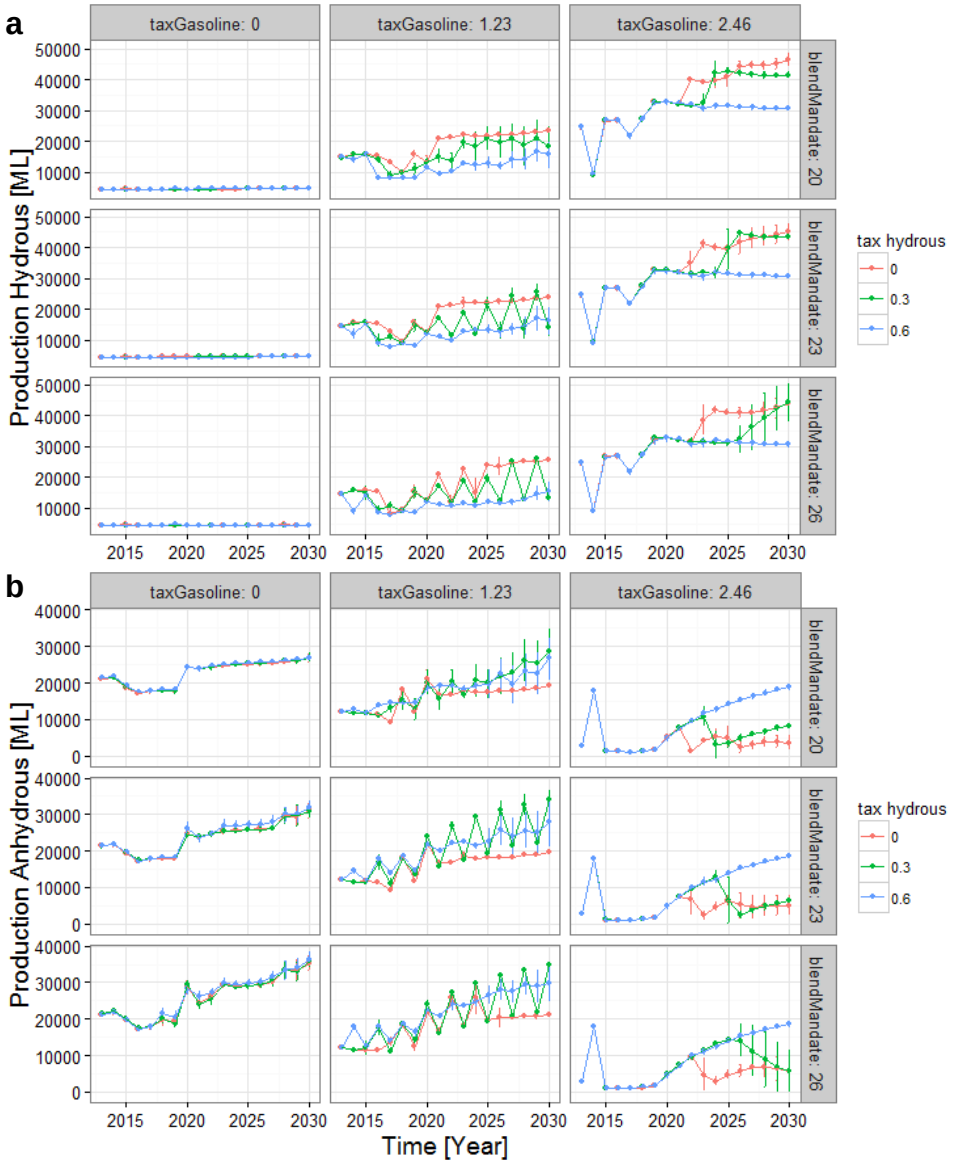

Figure E.9: Production of hydrous (**a**) and anhydrous ethanol (**b**) over time for different combinations of blend mandate and tax levied on gasoline and hydrous ethanol. Tax on gasoline and hydrous ethanol in $R\$l^{-1}$. Blend mandate in %v/v. Anhydrous tax = 0.1 $R\$l^{-1}$. Dots and err bars represent the mean and the standard deviation, respectively. Forty repetitions were carried out in the simulations for each combination of policy instruments.

F

BRAZILIAN BIOJET FUEL SUPPLY CHAIN: MAIN ALGORITHMS

This appendix presents an overview of the model narrative and describes some of the most important processes executed during the simulation. Figure F.1 describes the narrative of the model. Figure F.2 describes the process by which the price of sugarcane is determined. Finally, Figure F.3 describes the process by which the price of the biofuels is determined.

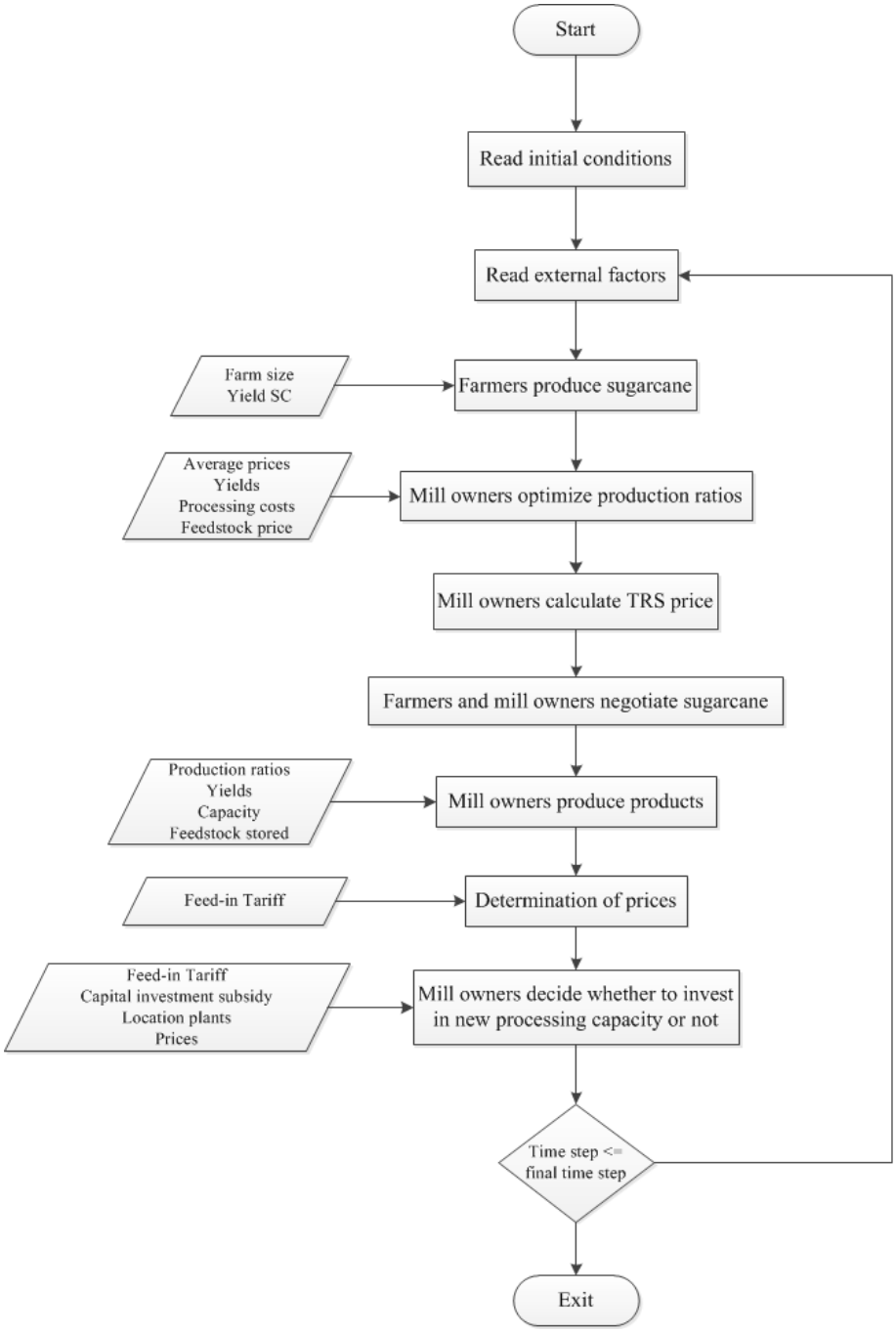

Figure F.1: Model narrative

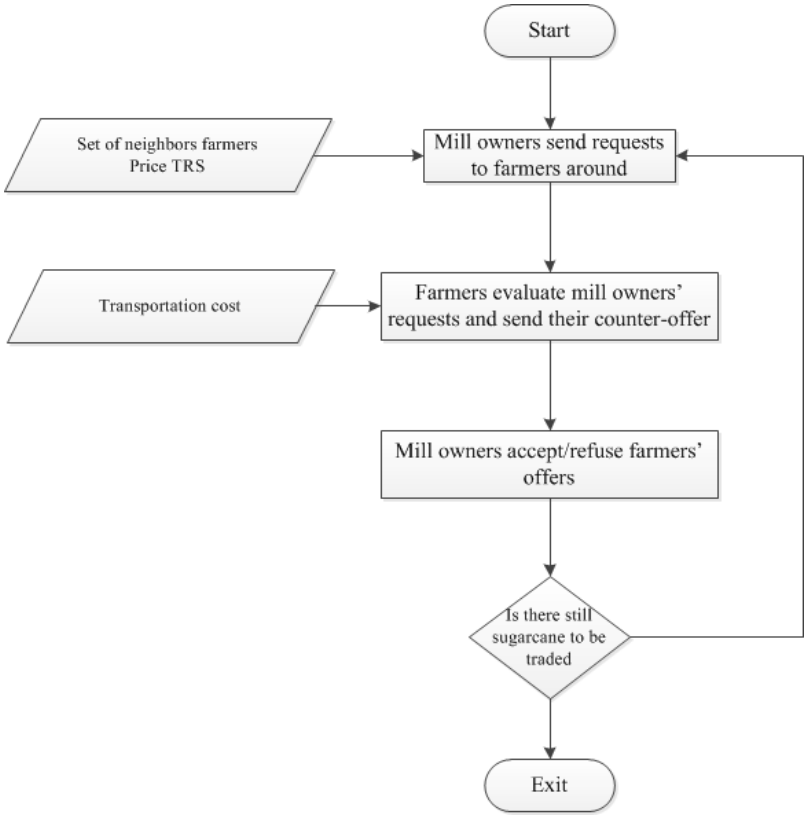

Figure F.2: Sugarcane negotiation

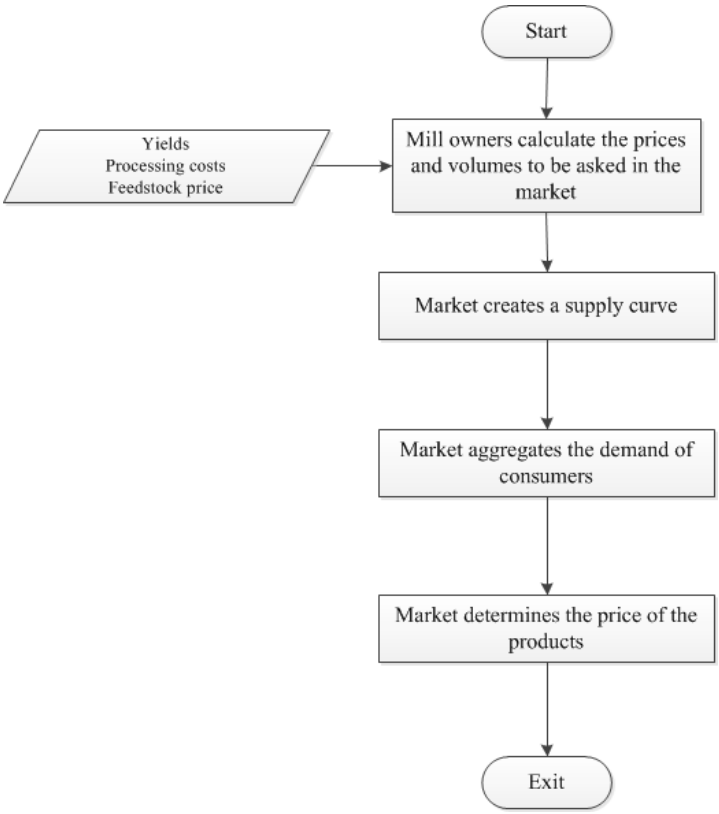

Figure F.3: Price determination

G

TECHNO-ECONOMIC DATA OF THE PRODUCTION OF BIOJET FUEL IN BRAZIL

This appendix describes the techno-economic data used in the calculation of the net present value. Table G.1 presents the fixed capital investment costs and processing costs for biojet fuel production. These costs include all the processing costs other than the feedstock cost.

Table G.1: Estimates of fixed capital investment costs and processing costs for biojet fuel production

Capacity	Sugar		Ethanol		Biojetfuel	
	Fixed Capital Investment[a]	Processing cost[b]	Fixed Capital Investment[a]	Processing cost[c]	Fixed Capital Investment[c]	Processing cost[c]
[Mt yr^{-1}]	[MUS$]	[MUS$ yr^{-1}]	[MUS$]	[MUS$ yr^{-1}]	[MUS$]	[MUS$ yr^{-1}]
1	32.05	8.84	32.13	8.88	16.59	20.56
3	69.16	26.52	101.83	26.64	33.89	61.79
5	98.89	44.19	173.02	44.44	47.23	103.02

[a] Based on the data reported in PECEGE[1]
[b] Based on the data reported in Jonker *et al.*[2]
[c] Based on the data reported in Santos *et al.*[3]

Production and financing assumptions are presented in Table G.2. The plant start-up schedule is presented in Table G.3.

[1] Production costs of sugarcane, sugar, ethanol and bioelectricity in Brazil:2014/2015 crop season and 2015/2016 crop projection. 2015, University of Sao Paulo, Luis de Queiroz College of Agriculture: Piracicaba. p. 73.

[2] Jonker, J.G.G., et al., Outlook for ethanol production costs in Brazil up to 2030, for different biomass crops and industrial technologies. Applied Energy, 2015. 147: p. 593-610.

[3] Santos, C.I., et al., Integrated 1st and 2nd generation sugarcane bio-refinery for jet fuel production in Brazil: Techno-economic and greenhouse gas emissions assessment. Renewable Energy, 2017.

Table G.2: Financing and production assumptions

Parameter	Value	Unit
plant lifetime	20	yr
installation time	3	yr
Income tax rate[a]	37	%
depreciation period	10	yr
discount rate[b]	U(10,20)	%
Price electricity[c]	250	$R\$\,MW^{-1}\,h^{-1}$

[a] Reference value for Brazil[4]

[b] Flex owners of flex plants differ in their perception of risk in the investment decision. Here, we use the discount rate as proxy for risk perception. The difference in risk perception among owners of flex plants was modeled by using a uniform distribution.

[c] Based on the data reported in ovoenergy[5]. The price was adjusted to take into account the losses of energy for distribution

Table G.3: Plant start-up schedule

Year	TCI schedule	Plant availability (% of capacity)
-2	33,33% Fixed Capital	0
-1	33,33% Fixed Capital	0
0	33,33% Fixed Capital	0
1		30
2		70
3		100

[4] Ives, C.M., et al., Techno-economic assessment of biorefinery technologies for aviation biofuels supply chains in Brazil. Biofuels, Bioproducts and Biorefining, 2017. 11(1): p. 67-91.

[5] Energy, O. Average electricity prices around the world: $/kWh. 2018; Available from: https://www.ovoenergy.com/guides/energy-guides/average-electricity-prices-kwh.html.

List of Publications

Peer-reviewed journal articles

- **Moncada, J. A.**, Lukszo, Z., Junginger, M., Faaij, A., Weijnen, M. *A conceptual framework for the analysis of the effect of institutions on biofuel supply chains.* Applied Energy, 185, Part 1. 2017. p. 895-915.

- **Moncada, J. A.**, Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *Exploring path dependence, policy interactions, and actor behavior in the German biodiesel supply chain.* Applied Energy, 2017. 195: p. 370-381.

- **Moncada, J. A.**, Park Lee, E. H., Nava Guerrero, G.D.C., Okur, O., Chakraborty, S.T., Lukszo, Z. *Complex Systems Engineering: designing in socio-technical systems for the energy transition.* EAI Endorsed Transactions on Energy Web, 2017, volume 3, issue 11.

- **Moncada, J. A.**, Verstegen, J. A., Posada, J.A., Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *Exploring policy options to spur the expansion of ethanol production and consumption in Brazil: an agent-based modelling approach.* Energy Policy, 2018. 123: p. 619-641.

Under review

- **Moncada, J. A.**, Verstegen, J. A., Posada, J.A., Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *Exploring the emergence of a biojet fuel supply chain in Brazil: an agent-based modeling approach.* Working paper submitted for publication (2018).

Conference proceedings

- **Moncada, J. A.**, Lukszo, Z., Junginger, M., Faaij, A., Weijnen, M. *A conceptual framework to analyze the co-evolution of institutions and biofuels markets.* Presented during the 24th European Biomass conference and Exhibition. Amsterdam - The Netherlands. June 6th - June 9th, 2016.

- **Moncada, J. A.**, Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *The role of institutions on the emergence of the German biodiesel supply chain: Exploring the path dependency and policy interactions.* Presented during the 24th European Biomass conference and Exhibition. Amsterdam - The Netherlands. June 6th - June 9th, 2016.

- **Moncada, J. A.**, Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *Agent-based model of the German Biodiesel Supply Chain.* Presented during the 12th PSE2015 and 25th ESCAPE. Copenhagen - Denmark. May 31st - June 4th, 2015.

- **Moncada, J. A.**, Junginger, M., Lukszo, Z., Faaij, A., Weijnen, M. *Analysis of the evolution of the biodiesel supply chain in Germany. An agent-based modelling approach.* Presented during the 23rd European Biomass conference and Exhibition. Vienna - Austria. June 1st - June 4th, 2015.

- Armbrust, T., **Moncada, J. A.**, van der Lei, T., Cunningham, S., van Stekelenburg, J., Weijnen, M. *Multi-agent simulation of the Brazilian bio-ethanol market.* Presented during the 23rd European Biomass conference and Exhibition. Vienna - Austria. June 1st - June 4th, 2015.

CURRICULUM VITÆ

Jorge Andrés MONCADA ESCUDERO

Jorge Andrés Moncada Escudero was born on 25 December 1982 in Puerto Salgar, Colombia. In 2006, he graduated with honors from the B.Sc. program in Chemical Engineering at National University of Colombia (UNAL) in Manizales. In 2009, he completed the M.Sc. program in Chemical Engineering at UNAL. He graduated cum laude for his thesis: *Application of thermodynamic concepts in the design and evaluation of reaction-separation processes for biodiesel production.* In the period 2008-2010, Jorge worked as a lecturer at UNAL and Caldas University on the subjects of separation processes design and fundamentals of heat transfer.

In 2011, he came to the Netherlands to pursue a Professional Doctorate in Engineering (PDEng) at Delft University of Technology. During this two-year program, he learned how to approach and solve real design problems using the engineering method, and how to work within an international team to address an industrial assignment.

In September 2013, he joined the faculty of Technology, Policy and Management at TU Delft and the Copernicus institute of sustainable development at Utrecht University as a Ph.D. researcher. He investigated the effect of policies and organizational structures on the deployment of biofuel supply chains. During his doctoral programme, Jorge published several peer-reviewed journal publications, supervised 4 master thesis projects, presented at 3 international conferences, and collaborated with other researchers. He was also a visiting Ph.D. student at the Centre for Environmental Policy at Imperial College London in the summer of 2016.

Since September 2018, Jorge began working as a postdoctoral fellow at Catholic University of Leuven. His current research interests include the use of (mathematical/agent-based) models to guide the transition of the energy system and support energy policy-making.