

Green Energy and Technology

Antonio Bonomi  
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Marco A.P. Lima *Editors*



# Virtual Biorefinery

An Optimization Strategy for Renewable  
Carbon Valorization

 Springer

# **Green Energy and Technology**

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Editors

# Virtual Biorefinery

An Optimization Strategy for Renewable  
Carbon Valorization

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ISSN 1865-3529

Green Energy and Technology

ISBN 978-3-319-26043-3

DOI 10.1007/978-3-319-26045-7

ISSN 1865-3537 (electronic)

ISBN 978-3-319-26045-7 (eBook)

Library of Congress Control Number: 2015953802

Springer Cham Heidelberg New York Dordrecht London

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Printed on acid-free paper

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# Foreword

I am pleased and honored to be asked to write the Foreword for this book on the Virtual Sugarcane Biorefinery (VSB) project. I first learned of the VSB about six years ago and have been keeping track of the project ever since through meetings with my friends at the University of Campinas (UNICAMP) and the Brazilian Bioethanol Science and Technology Laboratory (CTBE). I was excited by the initial concept, and am delighted to see how much progress has been made by the CTBE and UNICAMP teams in realizing their objectives. They should be proud of what they have accomplished.

The VSB is unique; there is literally nothing like it in all the world. The VSB project embraces all phases of this system, from the agricultural sector through the final use of the biorefinery products. Nowhere else in the world are the tools of economic, environmental, and social modeling being combined to improve an existing industry (sugarcane refining) while also laying the foundation to understand and improve the sustainability of an emerging industry: second-generation ethanol (and other products) from sugarcane cellulosic biomass. The goal of the VSB is to focus research and development and increase our understanding so that a new industry can arise to sustainably use all of the sugarcane plant; sucrose, bagasse, and leaf matter, in order to provide food, liquid fuel, electricity, and other products. What an ambitious and important goal. The CTBE/UNICAMP team is leading the world in applying the latest in systems modeling to shape the emergence of a new, sustainable industry. I believe the world will increasingly appreciate and be grateful for what you are doing. Personally, I express my deepest thanks and admiration to my dedicated and capable Brazilian colleagues. I am grateful for your leadership in this effort.

Muito obrigado!

Bruce E. Dale, University Distinguished Professor

Michigan State University

Editor in Chief: Biofuels, Bioproducts and Biorefining

The first decade of this century was a vigorous moment for science, technology, and innovation policy in Brazil. In parallel with a fast economic growth

characterized by a strong social inclusion policy focused on the expansion of the domestic consumer market, the federal government increased the amount of funds for research activities and, especially, for the development of some of the country's natural competitive advantages.

This book on the subject of virtual biorefinery brings illuminating lights on the development of such an important subject in Brazil and enumerates the country's remarkable achievements on the development of this technology platform on its several dimensions and potential applications. At that time, benefited by a 30 years' experience since the inception of the 1970s National Ethanol Program, Brazil had a worldwide leadership on the production and use of bioethanol. The country had already been recognized by international studies as a Natural Knowledge Economy, a qualification resulting not only from its strong natural resources base, but also from a growing scientific performance in the period.

Within such an environment, a study organized by the Center for Strategic Studies and Management on Science, Technology and Innovation (CGEE) had identified the principal bottlenecks for the full exploitation of the Brazilian advantages on bioethanol from sugarcane as a substitute for gasoline. CGEE, a think-tank of the Ministry of Science, Technology and Innovation, had been created in 2001 with the objective to develop key studies that incorporate different views and actors (academy, industry, and government) of the innovation system to support policy decisions. In this study, a complete strategy to promote the increase of ethanol production with the use of sugarcane as the most important renewable organic matter was designed. Its main conclusion was that the expansion of the Brazilian capability of exploring the whole sugarcane potential for large-scale and sustainable ethanol production would depend on the cumulative scientific and technological advances along the entire chain of ethanol production, which ranges from the agricultural fields to the industrial stage. It was also suggested that without a strong basic research program, the challenges associated with the development of second-generation technology (i.e., one that allows the complete use of the full organic matter present on sugarcane) could not be surmounted.

The final decision of the federal government was for the creation of a national laboratory for ethanol technology development (Brazilian Bioethanol Science and Technology Laboratory – CTBE), using the well-established model of open laboratory already in operation in other areas in Brazil. The CTBE was to bring together, in a strong collaborative manner, the research efforts under way at the academic and industrial segments, as well as developing its own expertise. An interdisciplinary team from different areas of knowledge, including researchers in biotechnology, chemistry, agriculture science, bioscience and modeling engineering, among others, was recruited to start the Brazilian national effort toward the development of second-generation technology for ethanol production. Due to the complexity and challenges to be faced, such effort would require strong national and international collaboration. Each chapter in this book presents a special contribution relating the necessary efforts required for a well-balanced advancement of the knowledge needed to support the wise strategy for technology and innovation followed in pursuing a sustainable energy future for humanity.

Lucia C. P. de Melo

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Energy policy is the continuation of war by other means and, only too frequently, the inverse is also true. The strategic, economic, financial, political, and social interests that determine and are determined by energy issues are at the core of the modern national industrial states. At the same time, and this is the reason we say energy policy is war pursued by other means, the consequences of the choices these nations make extrapolate their own borders. All sorts of international conflicts arise and become inevitable around energy issues. The fair number of international organizations, governmental or non-governmental, that exist to deal with these is a witness to their depth and breadth. In addition, over the past couple of decades, environmental issues, local and global, connected to the exploration of energy sources, transportation, transformation, distribution, and final uses of energy have become preeminent.

In 2015, we cannot say there is a global energy crisis, like the ones that occurred in the last decades of the twentieth century. The supply of fossil fuels is abundant and their prices are low. It is true that the world economy is not operating at full steam, and that we may be just experiencing one of those recurring moments in the economic cycle when supply overtakes demand. However, there is a latent energy crisis of another nature and almost unimaginable reach: anthropogenic global climate changes due to the emission of greenhouse gases into the atmosphere, mostly arising from the burning of fossil fuels. Global climate change, to the extent estimated by specialists and already partially indicated by real events, will have enormous negative economic and social consequences, especially from mid-twenty-first century onwards, that is, during the lifetime of the majority of human beings alive now. More and more, the questions appear to be not “if” there is trouble ahead, but “when, where, and how extensive, expensive and permanent” the damage will be. Dreams of a radiant future for mankind, of a poverty and disease free peaceful world, or more modestly, the digital utopia (the adjective delirious is superfluous) of bits and bytes prophets, are threatened by our undeniable success in securing, for the past two and a half centuries, abundant and cheap fossil energy supplies to power the modern industrial civilization.

The preceding paragraphs should underline the importance of the work reported in this book. The authors address in a systematic and quantified way the central question of the sustainability of biofuels. Biofuels are one of the several sources of renewable non-fossil energies that will have to be quickly deployed, if the worst consequences of global climate change are to be averted. The authors’ focus is on the virtualization of bioenergy transformation centers—biorefineries—in particular for sugarcane feedstocks. As defined in Chap. 2, “Biorefinery is a facility that integrates biomass conversion processes and equipment to produce fuels, power, materials and chemicals from biomass.” The novel simulation tools developed by the authors for the sugarcane biorefinery complement those available commercially for the chemical industry in general. More importantly, they cover the important

upstream agricultural processes and the downstream transportation process, taking the Brazilian case as their paradigm. This is, as the authors themselves recognize, a work in progress. They point out the limitations and the required (ongoing) research to increase the reliability and accuracy of the simulations. However, the book comes at the right time to draw attention to the tools already developed to help researchers quantify the impacts of sugarcane biofuels (and co-products), to evaluate quantitatively the consequences of the gigantic production scale-up required if bioethanol is to have a real impact on the market and on the reduction of the risks of global climate changes, and to guide policy and investment decisions. There is one aspect of the life cycle analysis that the authors do not address directly, that is, the energy and environmental costs for building, operating, and decommissioning a biorefinery. An interesting question is, for instance, what is the energy payback time of a biorefinery? These issues will become relevant if the production scale of sugarcane bioethanol is to increase by tenfold or more. I am sure that the question is already on the authors' To Do list.

The team at the Brazilian Bioethanol Science and Technology Laboratory (CTBE) and UNICAMP is to be warmly congratulated for the original and painstaking work of designing and implementing a virtualization tool for sugarcane biorefineries. They have produced a reference work of great value that deserves to be widely known and used.

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## Preface

In the early 2000s, the Americans started a heavy investment for replacing part of the gasoline, used in light vehicles, by ethanol produced from corn. The global renewable energy sector incorporated a strong ally. The Brazilians, with long tradition on using ethanol from sugarcane (at that time, about half of the fuel used in light vehicles in Brazil was ethanol), saw, in this action, great opportunities to their country. If the idea would spread around, new ethanol markets would open for their economically competitive product. In 2005, a government-hired agency, Center for Strategic Studies and Management—CGEE, linked to the Minister of Science, Technology, and Innovation, financed a study evaluating the possibility of busting up the Brazilian production, to a point of being able to replace 5–10 % of the worldwide gasoline consumption in 2025, by Brazilian sugarcane ethanol. This study [a summary is in “Can Brazil replace 5 % of the 2025 gasoline world demand with ethanol?” (Leite et al. 2009)] pointed out the bottlenecks in sugarcane agriculture, in ethanol industry, in the sustainability strategy, and on the needed basic science, composing a necessary agenda to be developed, in order to accomplish this goal. As a result, a National Laboratory on Ethanol was created, initially with four scientific and technological programs designed to attack the four bottlenecks areas of this ambitious plan. I was the first director and responsible for implanting it. As scientists, we know how to measure the success of a research program: follow the publications, the leadership, the publication citations, the upcoming scientific research lines, and so on. For measuring success in technological innovation, follow the money (patent profits). Unfortunately, for a National Laboratory that needs to accomplish goals on all the above-mentioned programs and foment lines of research, it is not possible to follow the basic science reasoning for success or wait for the profit stage to grant success in technological developments. We needed a strategy for making decisions in a day-to-day basis. For this, we have hired a senior researcher, Dr. Antonio Bonomi, with great experience in computer simulations for comparing different technological routes for ethanol production. His responsibility

in this new National Laboratory was to put a team together (the co-editors Dr. Cavalett and Dr. Cunha participate actively in this group) and run a Technological Assessment Program: the Virtual Sugarcane Biorefinery, a tool to link together all other programs and help the decision makers. This book is about this initiative—a strategy understood as an effective way to develop both science and technology looking for sustainable technological development.

Marco A.P. Lima

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# Acknowledgments

The authors would like to thank all those who have directly and indirectly contributed to the book and with the conception and development of the Virtual Sugarcane Biorefinery. Special mentions are to Rogério Cezar de Cerqueira Leite (University of Campinas and CNPEM), Luis Augusto Barbosa Cortez (University of Campinas), R. Maciel Filho (University of Campinas), Marcelo Zaiat (University of São Paulo), Carlos Alberto Labate (University of São Paulo), Carlos Eduardo Rossell (CTBE), Manoel Régis Lima Verde Leal (CTBE), Arnaldo Walter (University of Campinas), Marcos Buckeridge (University of São Paulo), Helena Chum (NREL), Guido Zacchi (Lund University), and Oscar Braunbeck (CTBE). Special recognition also for collaborators at CTBE and CNPEM, as well as the students and fellows who worked and have been working on Virtual Sugarcane Biorefinery. We thank all the present and past collaborators in the figures of Dr. Carlos Américo Pacheco (General Director of CNPEM), and Dr. Paulo Mazzafera (Director of CTBE). We acknowledge the Brazilian Center for Research in Energy and Materials (CNPEM); Ministry of Science, Technology and Innovation (MCTI); Coordination for the Improvement of Higher Education Personnel (CAPES); National Counsel of Technological and Scientific Development (CNPq), and São Paulo Research Foundation (FAPESP) for financial support for different parts of Virtual Sugarcane Biorefinery.

# Contents

<b>1 Background</b> . . . . .	1
Marco A.P. Lima, Antonio Bonomi, Otávio Cavalett and Marcelo Pereira da Cunha	
<b>2 The Virtual Sugarcane Biorefinery Concept</b> . . . . .	5
Antonio Bonomi, Otávio Cavalett, Marcelo Pereira da Cunha and Marco A.P. Lima	
<b>3 The Agricultural Production Model</b> . . . . .	13
Otávio Cavalett, Mateus F. Chagas, Paulo S.G. Magalhães, João L. N. Carvalho, Terezinha F. Cardoso, Henrique C.J. Franco, Oscar A. Braunbeck and Antonio Bonomi	
<b>4 Biorefinery Alternatives</b> . . . . .	53
Edvaldo R. Morais, Tassia L. Junqueira, Isabelle L.M. Sampaio, Marina O.S. Dias, Mylene C.A.F. Rezende, Charles D.F. de Jesus, Bruno C. Klein, Edgardo O. Gómez, Paulo E. Mantelatto, R. Maciel Filho and Antonio Bonomi	
<b>5 Biorefinery Products Logistics, Commercialization, and Use.</b> . . . . .	133
Mateus F. Chagas, Otávio Cavalett, Lucas Gonçalves Pereira and Antonio Bonomi	
<b>6 Sustainability Assessment Methodologies.</b> . . . . .	155
Marcos D.B. Watanabe, Lucas G. Pereira, Mateus F. Chagas, Marcelo Pereira da Cunha, Charles D.F. Jesus, Alexandre Souza, Elmer C. Rivera, R. Maciel Filho, Otávio Cavalett and Antonio Bonomi	

**7 Use of the VSB to Assess Biorefinery Strategies. . . . . 189**  
Marina O.S. Dias, Tassia L. Junqueira, Isabelle L.M. Sampaio,  
Mateus F. Chagas, Marcos D.B. Watanabe, Edvaldo R. Morais,  
Vera L.R. Gouveia, Bruno C. Klein, Mylene C.A.F. Rezende,  
Terezinha F. Cardoso, Alexandre Souza, Charles D.F. Jesus,  
Lucas G. Pereira, Elmer C. Rivera, R. Maciel Filho  
and Antonio Bonomi

**8 Use of VSB to Plan Research Programs and Public Policies. . . . . 257**  
Tassia L. Junqueira, Bruna Moraes, Vera L.R. Gouveia,  
Mateus F. Chagas, Edvaldo R. Morais, Marcos D.B. Watanabe,  
Marcelo Zaiat and Antonio Bonomi

**9 Final Remarks. . . . . 283**  
Antonio Bonomi, Otávio Cavalett, Marcelo Pereira da Cunha  
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# Abbreviations

.NET	Microsoft .NET Framework
1G	First-generation
1G2G	Integrated first- and second-generation
2G	Second-generation
ABE	Acetone, <i>n</i> -butanol, and ethanol
ABNT	Brazilian Technical Standards Association
Adv	Advanced technology
AFEX	Ammonia fiber expansion
ALC	Alcoholchemistry
ALO	Agricultural land occupation
Anfavea	Brazilian Automotive Industry Association
ANOVA	Analysis of variance
ANP	Brazilian National Agency of Petroleum, Natural Gas and Biofuels
Anx	Annexed plant
ASPEN	Advanced system for process engineering
Aut	Autonomous distillery
B30	Baling system for 30 % straw recovery
B50	Baling system for 50 % straw recovery
B70	Baling system for 70 % straw recovery
BDO	1,4-Butanediol
BG	Biogas
BIG/GT	Biomass integrated gasifier/gas turbines
BIG–GT/CC	Biomass-integrated gasification–gas turbine combined cycle
BM	Biomethane
Bio-PE	Biobased polyethylene
Brix (Bx)	Sugar content of an aqueous solution
BRL	Brazilian real
BS	Baling system
But	<i>n</i> -butanol

C <sub>12</sub>	Twelve-carbon sugar (sucrose)
C <sub>2</sub> H <sub>4</sub> eq	Ethylene equivalent
C <sub>4</sub>	Four-carbon molecule
C <sub>5</sub>	Five-carbon sugars (pentoses)
C <sub>6</sub>	Six-carbon sugars (hexoses)
CAPE	Computer-aided process engineering
CAPEX	Capital expenditures
CC	Conventional sugarcane
CCD	Central composite design
CCGT	Combined cycle gas turbine
CDM	Clean development mechanism
CER	Certified emission reduction
CETESB	Environmental Company of the State of São Paulo
CFC-11	Trichlorofluoromethane equivalent
CFD	Computational fluid dynamics
CH <sub>4</sub>	Methane
CHP	Combined heat and power
CIP	Cleaning in place
CNPEM	Brazilian Center for Research in Energy and Materials
CO	Carbon monoxide
CO <sub>2</sub>	Carbon dioxide
CO <sub>2</sub> -eq	Carbon dioxide equivalent
COD	Chemical oxygen demand
Cog	Cogeneration
COLaN	CAPE-OPEN Laboratories Network
COM	Component Object Model
CORBA	Common Object Request Broker Architecture
CTBE	Brazilian Bioethanol Science and Technology Laboratory
Cur	Current technology
DAE	Differential algebraic equation
DAP	Diammonium phosphate
db	Dry basis
DCOM	Distributed Component Object Model
DDGS	Dried distillers grains with solubles
DEHEMA	Society for Chemical Engineering and Biotechnology
DEPG	Dimethyl ethers of polyethylene glycol
DHFORM	Standard enthalpy of formation
DHSFRM	Solid standard enthalpy of formation
DME	Dimethyl ether
DNIT	Brazilian National Department for Transport Infrastructure
DOE	US Department of Energy
EC	Energy cane
EH	Enzymatic hydrolysis
EIA	US Energy Information Administration
EIO-LCA	Economic Input–Output Life Cycle Assessment

Elec	Electricity
EML	EMSO modeling library
EMSO	Environment for modeling, simulation, and optimization
EU	European Union
FDP	Fossil depletion
FT	Fischer–Tropsch
FT-SPK	Fischer–Tropsch synthetic paraffinic kerosene
FWEP	Freshwater eutrophication
GBL	<i>g</i> -Butyrolactone
GHG	Greenhouse gas
GLUCOLIG	Glucose oligomers
GMO	Genetically modified organisms
Gproms	General process modeling system
Grid	Electric grid
GWP	Climate change (global-warming potential)
HAP	Hydroxyapatite
HC	Henry component
HDPE	High-density polyethylene
HMF	Hydroxymethylfurfural
HTP	Human toxicity
I30	Integral harvesting for 30 % straw recovery
I50	Integral harvesting for 50 % straw recovery
I70	Integral harvesting for 70 % straw recovery
IC	Internal circulation
IEA	International energy agency
INPM	Mass ethanol percentage
IO	Input–output
IOA	Input–output analysis
IRR	Internal rate of return
IS	Integral harvesting system
ISO	The International Organization for Standardization
LCA	Life Cycle Assessment
LCF	Lignocellulosic feedstock
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCM	Lignocellulosic material
LDPE	Low-density polyethylene
LGNSOL	Soluble lignin
LHV	Lower heating value
LLDPE	Linear low-density polyethylene
LP	Low polarization
LPMO	Lytic polysaccharide monoxygenase
MAP	Monoammonium phosphate
MARR	Minimum acceptable rate of return or hurdle rate

MIT	Massachusetts Institute of Technology
MIXCINC	Conventional and nonconventional components
MMA	Brazilian Ministry of the Environment
MPI	Message passing interface
MPS	Brazilian Ministry of Social Security
MTBE	Methyl tert-butyl ether
MTC	Million tonnes of cane
MTE	Brazilian Ministry of Labor and Employment
n.a.	Not applicable
N <sub>2</sub> O	Nitrous oxide
NAE	Nonlinear algebraic equation
NC	Nonconventional components
NH <sub>3</sub>	Ammonia
NMHC	Non-methane hydrocarbons
NO <sub>3</sub> <sup>-</sup>	Nitrate
NO <sub>x</sub>	Nitrogen oxides
NPV	Net present value
NREL	National Renewable Energy Laboratory (USA)
NRTL	Non-random two-liquid model
NRTL-HOC	Non-random two-liquid activity coefficient model using the Hayden-O'Connell model for the vapor phase
Op	Optimized configuration
OpenMP	Open Multiprocessing
OPEX	Operational expenditures
P	Productivity
PACER	Process Assembly Case Evaluator Routine
PBS	Polybutylene succinate
P <sub>c</sub>	Critical pressure
PE	Polyethylene
PHA	Polyhydroxyalkanoate
PHB	Polyhydroxybutyrate
PLA	Polylactic acid
PM	Particulate matter
PM10-eq	Particulate matter equivalent (10 μm or less in diameter)
Pol	Apparent sucrose content
PR-BM	Peng–Robinson equation of state with Boston–Mathias alpha function
PREP-EXT	Preparation and extraction
PSD	Particle size distribution
PSE	Process Systems Enterprise
PVM	Parallel Virtual Machine
Q	Quadratic
QLC	Queensland low color
R&D	Research and development

R	Straw recovery fractions
RCHO	Aldehydes
RKS-BM	Redlich–Kwong–Soave cubic equation of state with Boston–Mathias alpha function
S	Scenario
SC	Sugarcane
SHF	Separate hydrolysis and fermentation
S-LCA	Social Life Cycle Assessment
SNA	System of national accounts
SO <sub>2</sub> -eq	Sulfur dioxide equivalent
SPK	Synthetic paraffinic kerosene
SSCF	Simultaneous saccharification and co-fermentation
SSF	Simultaneous saccharification and fermentation
SSP	Superphosphate
St	Standard configuration
STEAMNBS	Steam tables
TAP	Terrestrial acidification
Tb	Normal boiling point
Tc	Critical temperature
TC	Tonne of cane (sugarcane stalks)
The	Thermochemical 2G ethanol
THF	Tetrahydrofuran
Tkm	ton–kilometer
TRS	Total reducing sugars
TSP	Triple superphosphate
UASB	Upflow anaerobic sludge blanket
UK	United Kingdom
US\$	United States dollar
US	United States
USA	United States of America
V1	Bleed steam from first effect of multiple effect evaporator
V2	Bleed steam from second effect of multiple effect evaporator
VA	Value added
VHP	Very high polarization
VSB	Virtual sugarcane biorefinery
VVHP	Very very high polarization
WGS	Water-gas shift reaction
XYLOLIG	Xylose oligomers

# List of Figures

Figure 2.1	Basic principles of a biorefinery (based on Kamm and Kamm 2004). . . . .	6
Figure 2.2	General concept of the VSB . . . . .	7
Figure 3.1	Typical sugarcane production and transportation phases . . . . .	15
Figure 3.2	Agricultural model scheme showing different calculation modules . . . . .	17
Figure 3.3	Design of a Romeu e Julieta truck . . . . .	28
Figure 3.4	Design of a Treminhão truck . . . . .	28
Figure 3.5	Design of a Rodotrem truck . . . . .	29
Figure 4.1	Simple three-step biomass–process–product procedure (adapted from Fernando et al. 2006). . . . .	54
Figure 4.2	Whole-crop biorefinery block diagram (adapted from Kamm et al. 2006). . . . .	55
Figure 4.3	Green biorefinery block diagram (adapted from Kamm et al. 2006). . . . .	56
Figure 4.4	Lignocellulosic feedstock biorefinery block diagram (adapted from Kamm et al. 2006) . . . . .	57
Figure 4.5	Two-platform biorefinery block diagram (adapted from Kamm et al. 2006). . . . .	58
Figure 4.6	Range of biofuels and biobased chemicals obtained by catalytic conversion of biomass-derived syngas (adapted from Subramani and Gangwal 2008). . . . .	65
Figure 4.7	Simplified block diagram for the production of ethanol, sugar and electricity . . . . .	69
Figure 4.8	Products obtained from biomass thermochemical conversion . . . . .	78
Figure 4.9	Simplified block flow diagram for ethanol production using different feedstocks (adapted from BNDES and CGEE 2008). . . . .	83

Figure 4.10	General simulation program based on sequential modular approach (adapted from Raman 1985) . . . . .	84
Figure 4.11	Block flow diagram for an optimized annexed plant. . . . .	96
Figure 4.12	Process flowsheet for an optimized annexed plant . . . . .	98
Figure 4.13	Process flowsheet for fermentation section . . . . .	98
Figure 4.14	Block flow diagram for integrated 1G2G ethanol production . . . . .	104
Figure 4.15	Process flowsheet for second-generation process . . . . .	105
Figure 4.16	Convergence flowchart for process simulation. . . . .	108
Figure 4.17	Block flow diagram of the thermochemical conversion of sugarcane lignocellulosic material (LCM) to mixed alcohols . . . . .	109
Figure 4.18	AspenPlus diagram of the gasification (a) and tar reforming (b) sections of the thermochemical unit . . . . .	112
Figure 5.1	Typical Brazilian ethanol distribution system. . . . .	135
Figure 5.2	Ethanol distribution modeling scheme showing different calculation modules. . . . .	136
Figure 5.3	Fuel use modeling scheme . . . . .	148
Figure 6.1	Illustration of cost allocation for first- and second-generation ethanol. . . . .	161
Figure 6.2	A simplified schematic view of an economy . . . . .	163
Figure 6.3	A typical transactions table showing an economy aggregated in three sectors . . . . .	164
Figure 6.4	A simplified transactions table for Brazil in 2011 (billion Reais) . . . . .	165
Figure 6.5	Quantification of occupational accidents in the biorefinery supply chain based on the EIO-LCA framework ( $X$ is the vector of industry outputs; $(I - A)^{-1}$ is the Leontief Inverse; $Y$ is the vector of final demands; $R$ is the diagonal matrix of workers per dollar output, and $Z$ is the vector of accidents per worker) . . . . .	169
Figure 6.6	System boundaries considering a field-to-gate approach for the production of anhydrous ethanol and surplus electricity from sugarcane . . . . .	171
Figure 6.7	Structure of the system of equations (mixed technology approach) <i>Source</i> Watanabe et al. (2015) . . . . .	176
Figure 6.8	Examples of probability distributions . . . . .	179
Figure 6.9	Examples of results obtained in the risk analysis . . . . .	179
Figure 6.10	Scheme for the surrogate model construction for a the entire sugarcane production chain emulated by the VSB and b a subsystem of the VSB. . . . .	182
Figure 6.11	Example of a typical standardized Pareto Chart of three variables. The linear and quadratic effects are, respectively, denoted by $(L)$ and $(Q)$ . . . . .	184

Figure 7.1	Summary of results for first-generation annexed plants and autonomous distilleries (considering ethanol, electricity and sugar moving average prices over the last decade) . . . . .	197
Figure 7.2	Summary of results for 1G annexed plants and autonomous distilleries (considering ethanol, electricity and sugar average prices of July 2014) . . . . .	197
Figure 7.3	First-generation ethanol costs of annexed plants and autonomous distilleries (considering ethanol, electricity and sugar moving average prices over the last decade). . . . .	198
Figure 7.4	First-generation ethanol costs of annexed and autonomous distilleries: standard and optimized configurations (considering ethanol, electricity and sugar average prices of July 2014) . . . . .	198
Figure 7.5	Comparative environmental scores for ethanol production in standard and optimized scenarios of annexed plants and autonomous distilleries ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i> terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>FDP</i> fossil depletion) . . . . .	201
Figure 7.6	Breakdown of the environmental impacts of ethanol production for optimized autonomous distillery ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i> terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>FDP</i> fossil depletion) . . . . .	202
Figure 7.7	Breakdown of second-generation ethanol production costs . . . . .	207
Figure 7.8	Comparative environmental scores for ethanol production with current and 1G2G–Adv technologies ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i> terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>ALO</i> agricultural land occupation; <i>FDP</i> fossil depletion) . . . . .	208
Figure 7.9	Comparison of advanced stand-alone 2G and integrated 1G2G ethanol production costs . . . . .	211
Figure 7.10	Comparative environmental scores for ethanol production with integrated and stand-alone 2G ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i> terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>ALO</i> agricultural land occupation; <i>FDP</i> fossil depletion) . . . . .	212
Figure 7.11	Breakdown of the environmental impacts of stand-alone 2G ethanol production in 2G-Adv scenario ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i>	

	terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>ALO</i> agricultural land occupation; <i>FDP</i> fossil depletion) . . . . .	212
Figure 7.12	Block flow diagram for optimized autonomous distillery with sugarcane processing . . . . .	214
Figure 7.13	Block flow diagram for optimized autonomous distillery with sweet sorghum processing . . . . .	214
Figure 7.14	Block flow diagram for corn processing . . . . .	217
Figure 7.15	Block flow diagram for season period: sugarcane processing and 1G2G ethanol production . . . . .	218
Figure 7.16	Block flow diagram for off-season period: 2G ethanol production from sugarcane LCM . . . . .	219
Figure 7.17	Comparison of season (1G–Aut–Op) and off-season scenarios (1G–Sorghum, 1G–Corn and 1G2G–Adv). . . . .	221
Figure 7.18	Ethanol production costs considering different season and off-season configurations . . . . .	222
Figure 7.19	Comparative environmental impact scores for ethanol production in harvest extension scenarios ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>TAP</i> terrestrial acidification; <i>FWEP</i> freshwater eutrophication; <i>FDP</i> fossil depletion). . . . .	223
Figure 7.20	Breakdown of global warming potential shares for ethanol production in harvest extension scenarios. . . . .	224
Figure 7.21	Simplified block flow diagram of the sugarcane biorefinery producing <i>n</i> -butanol through ABE fermentation . . . . .	226
Figure 7.22	Simplified block flow diagram of the sugarcane biorefinery producing <i>n</i> -butanol through ethanol catalysis . . . . .	227
Figure 7.23	IRR values considering <i>n</i> -butanol and coproducts selling prices uncertainties. . . . .	230
Figure 7.24	Breakdown of second-generation ethanol production costs (US\$/m <sup>3</sup> ) . . . . .	235
Figure 7.25	Comparative environmental scores for ethanol production with biochemical and thermochemical 1G2G technologies ( <b>Note</b> <i>GWP</i> climate change; <i>HTP</i> human toxicity; <i>FWEP</i> freshwater eutrophication; <i>ALO</i> agricultural land occupation; <i>FDP</i> fossil depletion) . . . . .	235
Figure 7.26	Trends in the straw recovery costs for different fractions of straw recovery and transport distances. . . . .	240
Figure 7.27	Economic results of the vertically integrated scenarios considering different straw recovery systems. . . . .	241
Figure 7.28	Breakdown of electricity production costs (considering both operating and capital costs) . . . . .	242