Green Energy and Technology

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Marco A.P. Lima *Editors*

# Virtual Biorefinery

## An Optimization Strategy for Renewable Carbon Valorization

Springer

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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 illumining 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
Pernambuco State Secretary of Science, Technology and Innovation
Former President of the Center for Strategic Studies and Management on Science, Technology and Innovation—CGEE

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.

Cylon Gonçalves da Silva, Professor Emeritus
State University of Campinas—UNICAMP
Member of the Coordination for Special Programs, Scientific Directorate, FAPESP (São Paulo Research Foundation).

# 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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# Abbreviations

| | |
|---|---|
| .NET | Microsoft .NET Framework |
| 1G | First-generation |
| 1G2G | Integrated first- and second-generation |
| 2G | Second-generation |
| ABE | Acetone, *n*-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 | *n*-butanol |

| | |
|---|---|
| $C_{12}$ | Twelve-carbon sugar (sucrose) |
| $C_2H_4$eq | Ethylene equivalent |
| C4 | Four-carbon molecule |
| C5 | Five-carbon sugars (pentoses) |
| C6 | 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 |
| $CH_4$ | Methane |
| CHP | Combined heat and power |
| CIP | Cleaning in place |
| CNPEM | Brazilian Center for Research in Energy and Materials |
| CO | Carbon monoxide |
| $CO_2$ | Carbon dioxide |
| $CO_2$-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 |
| DECHEMA | 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 | *g*-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 monooxygenase |
| MAP | Monoammonium phosphate |
| MARR | Minimum acceptable rate of return or hurdle rate |

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|---|---|
| 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 |
| $N_2O$ | Nitrous oxide |
| NAE | Nonlinear algebraic equation |
| NC | Nonconventional components |
| $NH_3$ | Ammonia |
| NMHC | Non-methane hydrocarbons |
| $NO_3^-$ | Nitrate |
| $NO_X$ | 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 phas |
| Op | Optimized configuration |
| OpenMP | Open Multiprocessing |
| OPEX | Operational expenditures |
| P | Productivity |
| PACER | Process Assembly Case Evaluator Routine |
| PBS | Polybutylene succinate |
| Pc | 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 |
| SO2-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