

## Chapter 2

# The Virtual Sugarcane Biorefinery Concept

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Biorefinery is a facility that integrates biomass conversion processes and equipment to produce fuels, power, materials, and chemicals from biomass. The biorefinery concept is analogous to today's petroleum refineries, which produce multiple fuels and products from fossil oil. Industrial biorefineries have been identified as the most promising routes for the creation of a new domestic biobased industry (Kamm et al. 2006). Figure 2.1 shows a general scheme of biorefinery concept.

The Brazilian Bioethanol Science and Technology Laboratory (CTBE), one of the four National Laboratories that integrate the National Center for Research in Energy and Materials, was inaugurated by the Ministry of Science, Technology and Innovation of the Brazilian Government in 2010. The aim of CTBE foundation is to contribute in deepening the Brazilian leadership in the sectors of renewable energy sources and chemical industry raw material production, mainly by improving the sugarcane bioethanol production chain, through research, development, and innovation, integrating the productive sector and the Brazilian scientific-technology community.

Since the beginning of CTBE's construction, it was conceived that the idea of developing a "tool" (i.e., an applied methodology) that would allow comparing different technological routes and would contribute for the decision-making process.

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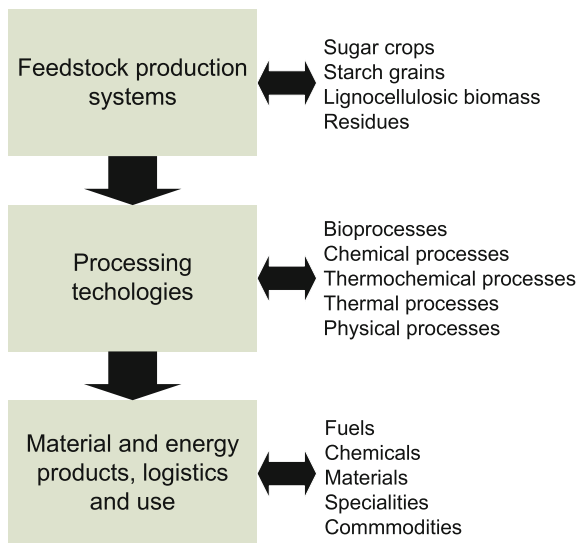
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**Fig. 2.1** Basic principles of a biorefinery (based on Kamm and Kamm 2004)



This technological assessment tool emerged from the need of setting a methodology to measure CTBE's success. With this purpose, the construction of a simulation tool was designed—the Virtual Sugarcane Biorefinery (VSB). A plan containing the idea, objectives, scope, and methodology for the VSB construction was submitted, evaluated, and approved by the bioethanol and sugarcane community (including academy and industry) in the workshop “VSB: Assessing success of new technologies,” organized by CTBE in 2009.

The VSB is a simulation platform that allows the evaluation of the integration of new alternatives for the sugarcane sector—cellulosic ethanol and other products from the green chemistry in the biorefinery concept, new agricultural strategies for sugarcane production, as well as different strategies for ethanol and other products used as biofuels and biochemicals. In a first approach, technologies adopted today in the whole sugarcane production chain are used as reference for this evaluation. The results obtained with the VSB have been validated against existing plants or results from laboratory or pilot scales available experiments for the new technologies, in order to guarantee the accuracy of the sustainability impacts calculated with this simulation tool.

The VSB has also been used to assess the level of success reached by CTBE's Pilot Plant for Process Development in the development of new industrial technologies in the biorefinery concept, as well as the CTBE's Agriculture Program innovations.

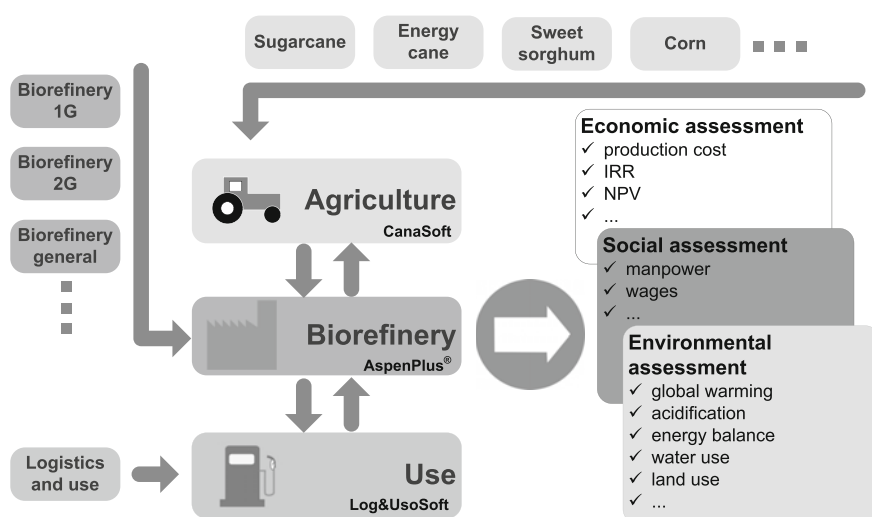
This tool also considers the logistics and use of biorefinery products, therefore including their entire production and consumption chain. Methodologies used for the assessment are identified and developed together with the sustainability experts at CTBE.

Therefore, from the above-described features of the VSB, it is clear its importance as a tool for the continuous evaluation and improvement of CTBE's research activities, as well as to evaluate the potential of several possible alternatives and technologies covering all aspects of the program. Summarizing, the VSB strategy aims at developing an analysis tool for sugarcane biorefineries, including the agricultural, industrial, and product-use sectors, which will make it possible to:

- optimize the concepts and processes included in a biorefinery;
- assess different biorefinery alternatives referring to their sustainability impacts (economic, environmental, and social); and
- assess the stage of development of the new technologies included in the analysis.

The VSB is based on mathematical modeling and simulation of different processes and operations included in the sugarcane production chain (agricultural, industrial, and usage sectors), which allow the estimation and optimization of the economic, environmental, and social impacts obtained with the new technologies under development. These results allow assessing the stage of development of new technologies, as well as the interest in accelerating the implementation process, orienting the laboratories participating in the development, about possible optimum operating conditions, and looking for their experimental confirmation.

The development of models and the use of computational tools (including specific commercial software) make it possible to assess the impacts of new technologies on the Brazilian bioethanol production chain in the three pillars of the sustainability. Figure 2.2 illustrates the general concept of the VSB. Methods used for the sustainability assessment are summarized below and detailed in Chap. 6.



**Fig. 2.2** General concept of the VSB

- **Economic:** Required investment, profitability (internal rate of return (IRR), net present value (NPV), and other parameters), revenues, production costs, and minimum selling prices of products and taxes among other parameters and their implications in the production chain are evaluated using economic engineering tools. At the same time, the sensitivity analysis of the most important technical parameters included in the technologies under development and test on the related costs and investments is performed, as well as a risk analysis related with the implementation of the new technologies.
- **Environmental:** Energy balance (relation between the renewable energy produced and the fossil energy consumed), greenhouse gas emissions balances, water consumption, and other environmental impacts included in the Life Cycle Assessment (LCA) methodology such as acidification, photo-oxidant formation, nitrification, eutrophication, and human toxicity are evaluated. New concepts and models such as land-use changes and improved methods for environmental impact assessment are being introduced in the environmental analysis of bio-fuels and biochemicals.
- **Social:** Some local impacts derived from the automation, plant scale, agricultural sector mechanization, among others, on the number and quality of created jobs (number of workers, occupational accidents, wages, and education profile), as well as land use, social relations with the community, and labor qualification are assessed. These impacts are established using a hybrid approach integrating Social Life Cycle Assessment (S-LCA) methodology and Input–Output Analysis (IOA). These economic models allow for the quantification of the changes in the activity level of each sector of the economy as a function of modifications on demand for products of one or more sector. The major advantage of the use of this hybrid methodology is the possibility of including the evaluation of indirect impacts that are normally unassessed in general Social Life Cycle methodologies.

The scope of the framework described and applied in this book is the construction/adaptation of a simulation platform aiming at helping the modeling, optimization and technical, socioeconomic and environmental assessment of integrated processes, major characteristic of a biorefinery, together with all the stages of the sugarcane production chain. This platform will help to identify the processes and parameters showing major economic, social, and environmental impacts, in order to help in the prioritization of the scientific and technological researches, as well as to help in the formulation of public policies.

A continuous improvement in several aspects of VSB fundamentals, including detailed models development and validation of databases, is fundamental for its use and acceptance for the different stakeholders involved in the process (government officials, industry, and researchers). For this purpose, it is clear that financial support is required and should be provided by projects with industry and governmental support.

## 2.1 Agricultural Sector

VSB defines alternatives and includes the simulation of the agricultural operations required to produce and make the biorefinery feedstock—mainly the sugarcane, among alternative feedstock, available to the industry. These operations can be synthetically described as follows:

- preplanting operations;
- soil preparation;
- manual or mechanical planting;
- cultivation—sugarcane plant and ratoon;
- manual or mechanical harvesting; and
- sugarcane transport.

In order to evaluate the technical, socioeconomic, and environmental impacts of different technological scenarios, an agricultural spreadsheet-based model (including a detailed description of the above-mentioned operations), named “CanaSoft” was constructed, validated, and integrated to the simulation tools used to represent the other sectors of the sugarcane production chain (a detailed description of this platform is presented in Chap. 3).

## 2.2 Industrial Sector

In order to make the inclusion and the sustainability assessment of several biorefinery alternatives viable, it is necessary to define and technically evaluate different proposals and routes to transform biomass into products. The VSB focuses on sugarcane as the biomass to be used and the first- and second-generation bioethanol as the major product. It includes the analysis of other products such as sugar, electricity, other liquid fuels (obtained using the thermochemical route to convert the lignocellulosic material), materials (such as the polyhydroxyalkanoates obtained through sugars fermentation), and primers for the chemical industry (obtained from ethanol, sugar, or fractions of the lignocellulosic material), among others.

Therefore, some basic routes were designed and technically assessed, being a basis for the construction of the VSB, always using sugarcane as the major feedstock.

The simulation platform represents the different basic routes proposed in the construction of the VSB. Several commercial packages are available in the market, which are oriented to process simulation. ASPEN Plus ([www.aspentech.com/products/aspentech-plus.aspx](http://www.aspentech.com/products/aspentech-plus.aspx)), SuperPro Designer ([www.intelligen.com/superpro\\_overview.html](http://www.intelligen.com/superpro_overview.html)), and EMSO ([www.enq.ufgrs.br/trac/alsoc/wiki/EMSO](http://www.enq.ufgrs.br/trac/alsoc/wiki/EMSO)) are just some possibilities of commercial simulation packages. They were developed for a large spectrum of industries: oil, petrochemicals, pharmaceuticals, biotechnologies, fine chemistry, mineral processing, microelectronic, and effluent treatment, among

others. For several reasons, which will be detailed in the topic related to the construction of the industrial sector of the VSB, Aspen Plus was selected as the platform for this simulation (a detailed description of the most important process simulations is presented in Chap. 4).

## 2.3 Logistics and Use Sectors

In order to complete the sugarcane production chain, the last sector to be simulated is the one that includes operations of commercialization and use of the different products produced in the biorefinery. If, for example, the ethanol is considered as the product to be assessed, the major operations to be considered for the simulation are as follows:

- transport of ethanol to/among the commercialization agents;
- mixture with gasoline (gasohol alternative); and
- final use (end of life) of ethanol in the vehicles.

A spreadsheet-based model so-called Log&UseSoft was constructed detailing the operations involved with logistics, considering different transportation distances and modes; use, considering the product exercising a function; and end of life, considering the emissions and final disposal, of the different products of a biorefinery, allowing for the assessment of the sugarcane production chain completely (a detailed description is presented in Chap. 5).

Finally, it is clear that three development versions of the VSB are defined in order to characterize the quality and accuracy of the simulation performed during the use of the VSB for the assessment purposes. The descriptions of these versions are illustrated for the industrial sector, but they can be applied, with minor adjustments, to the other sectors of the production chain.

- **Preliminary Version:** All the simulations are performed based on preliminary flow diagrams and, in general, using data available in the literature.
- **Consolidated Version:** All the simulations are performed based on a conceptual design performed for the assessed technology or using operation description discussed in detail with specialists, when the other sectors of the chain are considered.
- **Validated Version:** The parameters used in the simulation are compared with the results obtained using data measured or obtained in commercial operations. Generally, three levels of validation, validated against one technology, validated against different technologies, and validated against different technologies and regional conditions, are considered.

The VSB has been successfully applied to compare different technological scenarios from government (public policies) and business aims, as well as to evaluate research bottlenecks to be prioritized. For instance, the VSB was used to perform a comprehensive assessment of evolution of 2G ethanol technologies in

time to estimate the learning curve of 2G ethanol cost. These results were validated against dozens of stakeholders. The study counted with participation of the Brazilian Development Bank (BNDES), and it is a great example of the use of VSB for promoting public policies, considering and defining priorities and performing a periodic evaluation of the research progress (Milanez et al. 2015).

The VSB has also been used in several technology development projects in collaboration with companies, performing a periodic evaluation of the research achievements and directing efforts in the research and development.

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An Optimization Strategy for Renewable Carbon  
Valorization

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(Eds.)

2016, XL, 285 p. 83 illus., Hardcover

ISBN: 978-3-319-26043-3