Multi-scale process and supply chain modelling: from lignocellulosic feedstock to process and products

Seyed Ali Hosseini¹ and Nilay Shah²,*

¹Department of Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK
²CPSE, Department of Chemical Engineering and Chemical Technology, Imperial College, South Kensington, London SW7 2AZ, UK

There is a large body of literature regarding the choice and optimization of different processes for converting feedstock to bioethanol and bio-commodities; moreover, there has been some reasonable technological development in bioconversion methods over the past decade. However, the eventual cost and other important metrics relating to sustainability of biofuel production will be determined not only by the performance of the conversion process, but also by the performance of the entire supply chain from feedstock production to consumption. Moreover, in order to ensure world-class biorefinery performance, both the network and the individual components must be designed appropriately, and allocation of resources over the resulting infrastructure must effectively be performed. The goal of this work is to describe the key challenges in bioenergy supply chain modelling and then to develop a framework and methodology to show how multi-scale modelling can pave the way to answer holistic supply chain questions, such as the prospects for second generation bioenergy crops.

Keywords: network design; supply chain modelling and planning; multi-scale modelling; future challenges

1. INTRODUCTION

Biofuels have been the object of intensive research and development since the energy crisis of the 1970s. A number of environmental and economic benefits are attributed to biofuels, such as energy security, reduction of greenhouse gas (GHG) emissions and availability of a storable renewable energy source for increasing energy demands. In addition, over the past few years, there has been an increasing awareness and acceptance of biofuels as a viable potential substitute for petroleum. It should be mentioned that the global economic downturn offers an opportunity to invest in green technology while costs and interest rates are lower. Furthermore, Wilkerson [1] provides a comprehensive study to show that green supply chain management (SCM) in not just about being environmentally friendly and in fact, it is a business value driver and not a cost centre. Thus, the authors of this study believe that green growth is the only realistic future for growth and overcoming world poverty.

However, the International Food Policy Research Institute claimed that the expansion of new sources of biofuels, such as ethanol, has had a strong effect on agricultural prices, since biofuel production currently draws largely on natural vegetation [2]. Biofuel production may have both direct and indirect effects on food prices; the direct effects may simply be the increasing demand for the ‘feedstock’, or the grain that feeds the plant, while the indirect effects of biofuel production will be more difficult to quantify and still remain to be seen. One such indirect claimed effect of bioethanol production in the US has been an increase in the feedstock price itself, and rising feedstock prices, in turn, have affected the prices of other grains. Higher prices for feedstock may cause food consumers to shift from to production of other grains that may result in dramatic side effects on both demand and supply. These demand- and supply-side effects have tended to increase the volatility of commodity market, which is directly related to global food security [3]. As a consequence, the potential impact of a large global expansion of biofuel production capacity on net food producers and consumers presents challenges for food policy planners, and raises the question of whether sustainable development targets at a more general level can ever be reached [4].

Changes in land use and combustion of fossil fuels are responsible for the greatest human impacts made on the global carbon cycle [5]. It has been claimed that bioenergy will reduce net GHG emissions. However, the GHG implications of energy production from biomass are more complex than the GHG implications of energy production from fossil fuels, since the carbon in biofuels is already part of the active global carbon cycle in which carbon exchanges rapidly between the
atmosphere and the biosphere. Bioenergy production does not add new carbon to the active carbon cycle, but it can affect global GHG levels in some important ways [6]. As shown in figure 1, land use change incurs GHG releases, usually referred to as ‘carbon debt’, and it is believed that based on the specific ecosystem involved, the carbon produced by biofuel consumption will return to ‘carbon stock’. The duration for this cycle is usually referred as the ‘payback period’, which is estimated to be between 100 and 1000 years [7]. Two mechanisms for land use change exist: ‘direct’ land use change, in which the land use change occurs as part of a specific supply chain for a specific biofuel production system, and ‘indirect’ land use change, which is harder to quantify and subject to considerable debate.

Although the main global concerns about biofuel are currently limited to sustainability, energy security and prices, each specific biofuel production facility also faces a wider range of uncertainties, such as which of different processes to choose, which feedstock will be best for the plant and even the best location for the plant, since all these factors are the main factors that determine cost. In addition to direct cost-determining factors, there are number of indirect effects, such as the effect of the production site and feedstock fields on local communities and the social economy.

Adequate literature exists about different aspect of green SCM and design [8]. Zhang et al. [9] provide a comprehensive literature review on the concept of green design, production scheduling and control for remanufacturing is discussed in great detail by Bras & McIntosh [10] and Guide & Daniel [11]. Issues regarding logistics network design for green manufacturing were studied by Fleischmann et al. [12,13] and Jayaraman et al. [14]. Zhu & Geng [15] deal with related areas of green purchasing, in addition sufficient literature also exist on industrial ecosystems and ecology [16–21].

Regarding integrated bioenergy supply chain models, Morrow et al. [22] developed a supply chain model of production and distribution of bioenergy from energy crops in the US using linear programming. They concluded that if ethanol is to be competitive in the long run, then in addition to process efficiency improvements, more efficient transportation infrastructure will need to be developed, such as pipelines. Yu et al. [23] presented a discrete mathematical model of mallee biomass supply chain in Western Australia; they came to the conclusion that transport, including on-farm haulage and road transport, can make significant contributions to the total cost of mallee biomass delivered to a bioenergy plant, then they recommended three strategies for reducing the delivered cost of mallee biomass namely: locating the biomass processing plant near areas of high planting density; better planning of seasonal schedules and integration of road transport into the business of either biomass growers or biomass processing plant owners.

Although all these earlier works provide a great insight into specific fields, they all have a narrow perspective and do not cover sufficiently all the aspects of bioenergy supply chain. In addition, most of the literature is empirical and there is a relative lack of integrated research on issues related to modelling and network design. Seuring & Müller [24] provided an in-depth literature review on sustainable SCM and argued that research is still dominant by green and environmental issues and research on integration of different aspects of bioenergy supply chain holistically is still rare.

There is a large body of literature describing the choice and optimization of different processes for converting feedstock to biofuels and bio-commodities. Sutton et al. [25] provide a comprehensive review of different gasification techniques, Quaak et al. [26] give an in-depth analysis of biomass combustion processes and Mohan et al. [27] reviewed various pyrolysis processes of biomass for bio-oil production. Issues regarding enzymatic hydrolysis of biomass are the subject of comprehensive review by Zhang & Lynd [28]. Mosier et al. [29] provide an in-depth review to show how the composition and sourcing of feedstock may affect the choice of different biomass pretreatment techniques prior to enzymatic hydrolysis. However, there is no single best process for all the different feedstocks and based on the source and composition of the

Figure 1. Overview of biorenewables life cycle.
feedstock, there may be several feasible processes [30]. The availability of the right feedstock for the conversion facility is a spatial function of crop production yields, land availability, rainfall and even the political decisions of local governments. Hence, all the determining factors for any specific biorefinery are interlinked, and that obtaining the maximum profit for a production site and the maximum benefit for the social economy is only possible by realizing the holistic nature of all the factors and their interrelationship at different scales. This in turn implies that the eventual cost of biofuel production will be determined not only by the performance of the conversion process, but also by the performance of the entire supply chain from feedstock production to end product use. These relationships can be explained through multi-scale modelling.

2. MULTI-SCALE MODELLING

Developing a holistic model for lignocellulosic bioconversion requires the incorporation of models from different fields, starting from systems biology to supply chain modelling. The integration of several parts of the bioenergy supply chain, as shown in figure 2, will give rise to a number of challenges, ranging from metabolic pathways to integration of planning, scheduling and control as well as the integration of measurements, control and information systems.

The properties of multi-scale systems critically depend on important behaviours coupled through multiple spatial and temporal scales, often without a clear separation between them, and as such, their description does not fall within the set of classical methods for crossing scales. Unfortunately, the ability to simulate complete systems does not follow immediately from an understanding of the component parts. Therefore, we need to know and model how the system is connected and controlled at all levels. Nevertheless, multi-scale modelling is the key to answering all the uncertainties in the bioenergy life cycle, since these uncertainties in nature arise from different time and length scales.

3. MULTI-SCALE PROCESS MODELLING AND THE SUPPLY CHAIN

There is a large body of literature regarding the choice and optimization of different processes for converting feedstock to biofuels and bio-commodities; moreover, there has been some reasonable technological development in bioconversion methods over the past decade (e.g. [31–33]). However, a question that has gone unconsidered in the literature is how technological developments in processing technologies and the life cycle of bioethanol feedstocks will affect the structure of the supply chain.

Shah [34] has divided all supply chain problems into three categories: (i) supply chain infrastructure (network) design; (ii) supply chain analysis and policy formulation; (iii) supply chain planning and scheduling. Bioenergy supply chain issues based on this classification are studied later below. Regarding bioenergy, there is a lack of methodology on how to incorporate all the available knowledge into one interconnected network to answer important supply chain questions. Some of the critical questions regarding bioenergy supply chain based on three classifications of supply chain issues are shown in table 1.

The key goal of this work is to develop a framework and methodology to show how multi-scale modelling can pave the way to answer holistic supply chain questions. This methodology shows how modellers should work alongside scientists engaged in fundamental experimental work on biomass production and conversion. Experimental work can be performed more
efficiently by model-based experimental design taking into account the interrelationship at different scales; this is illustrated in figure 3.

### 3.1. Supply chain network design

In the process system engineering (PSE) community, supply chain network design generally refers to broad strategic activities used to make decisions, such as location of production and storage, sourcing and allocation as well as choice of production process. Most of the time, models are employed to exploit potential trade-offs [34–37]. The bioenergy supply chain network is a direct medium for engaging the end users of biofuels and derivatives and the suppliers of the feedstock; thus, at first glance, the main data required for designing such a network is spatial distribution of biomass supply and energy (fuel, electricity and heat) demand. A great deal of the PSE literature deals with how to handle demand uncertainty, mainly for consumer products [38]; however, current global biofuel production, specifically in the European Union, is much lower than the desired target. Consequently, at this stage, research focused on demand forecasting is irrelevant as supply is far lower than current demands. In modeling terms, the authors believe that at this stage, demand should be treated as a deterministic temporally growing spatial function, and not as stochastic.

Classically, location–allocation problems have tended to focus only on logistical aspects [39,40]; however, in the process industry supply chain, greater benefits could be achieved by considering logistic and processing aspects simultaneously. The first step in the biofuel supply chain network design should be listing all the possible
bioconversion methods for any given biomass, together with a spatial representation of bioresource potential. Then, for any specific bioconversion method, a multi-period spatial optimization can be built to maximize the total net profit of global network and/or GHG and/or energetic efficiency. This type of model is usually based on technology capital and operating cost as well as distance, capacity and costs of biomass and ethanol; table 2 shows one example of the decision spaces for two processing options and three feedstocks. If there are a number of different types of objective functions (e.g. economics and environmental impacts) and trading off between these objectives is difficult, a multi-objective optimization procedure should be used. Considering these elements together provides opportunities for systems involving distributed pre-processing coupled with centralized processing [41].

In the optimization problem, key decision variables can be: mode of transport at each stage, operating mode of equipment in each time period, production and supply of products, number of echelons, number of components in each echelon and the connectivity between components in adjacent echelon. The choice of deciding factors usually depends on the availability of data and the complexity of the network; nevertheless, a larger number of decision factors usually lead to more robust network structures, although it makes the optimization problem more complex. In general, there exists a trade-off between model precision and complexity; thus, a modeler’s skill lies in choosing the right combination.

Having developed optimization problems for each specific biomass type and any possible bioconversion methods, one can then easily compare these networks based on metrics such as cost, GHG, capacity, products, etc. In this way, a supply chain network design can be a valuable tool for decision-making.

### Table 2. Example of the decision spaces for two processing options and three feedstocks.

<table>
<thead>
<tr>
<th>process</th>
<th>net profit</th>
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<tbody>
<tr>
<td>pyrolysis for corn stover</td>
<td>net profit = F(transportation cost, process operating and capital cost, processing time, temperature and pressure)</td>
</tr>
<tr>
<td>enzymatic hydrolysis for energy crops</td>
<td>net profit = F(transportation cost, process operating and capital cost, enzyme yield, enzyme cost, enzyme deactivation rate, processing time, temperature and pressure)</td>
</tr>
<tr>
<td>hybrid process for a mixture of corn stover, energy crops and forest residue</td>
<td>net profit = F(transportation cost, process operating and capital cost, enzyme yield, enzyme cost, enzyme deactivation rate, processing time, temperature and pressure, relative capacity, composition of mixture)</td>
</tr>
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</table>

3.1.2. Integration of process models and supply chain models. It should be mentioned that in the field of operational research and PSE, a very large amount of work has been undertaken to address both the infrastructure network design problem and the optimization of established networks. However, in most of the work to date, the potential benefit of including more detail in the manufacturing process has not been established. Since there is huge uncertainty regarding the efficiency of each bio-refining process option in its mature state, at this stage of development these uncertainties should be captured in the global network model, to direct the research in way that most benefits the global network. For example, Hosseini & Shah [31] showed that optimizing the biomass chip size in a dilute acid pretreatment process achieves average savings equivalent to a 5 per cent improvement in the yield of the biomass-to-ethanol conversion process. This kind of improvement in processing efficiency can lead to completely different result in global network optimization results; therefore, it is of utmost importance to formulate a methodology incorporating process uncertainty in the global supply chain network.
Although multi-scale modelling is a promising technique for integrating all processing aspects at different scales into the biofuel supply chain, computational efficiency is also an intellectual challenge in the PSE area, as computation usually increases exponentially with problem size [43]. One practical way to address this challenge would be to use conceptual process models from the molecular level up to the unit operation level in order to predict the possible range of operation and efficiency at each unit of operation, and then, in the supply chain model, consider the overall process as a combination of different outcomes, i.e. scenarios from process models at all scales. In other words, it would use characteristic models to run detailed dynamic simulations for each unit operation, and then use the results of these simulations (as ‘metamodels’) in the global network model offline. In this way, it would be possible to consider uncertainty at a process level in the supply chain model; moreover, since these uncertainties are determined by conceptual models, it would be possible to find the root of the uncertainties. For example, if the model predicts a rising cost—purity curve for a specified unit of operation, then it would be possible to integrate this into the supply chain model and choose the appropriate purity for that specific unit of operation in order to maximize the overall network efficiency. Therefore, in this approach, instead of considering the process as a black box, it would be possible to consider the process as a set of black boxes (unit operations) with a range of inputs and outputs for each unit of operation. Indeed, this approach would aid in optimizing the interactions between all available unit operations so that opportunities for new flowsheet configurations are facilitated.

As a precursor to this type of model integration, Dunnett et al. [41] describe how supply chain configurations for lignocellulosic ethanol may change as biomass production yields and conversion efficiencies increase. They noted that there are opportunities to exploit economies of scale in processing by, for example, employing crude ethanol pipelines if fermentation titres continue to increase.

3.2. Supply chain simulation

Simulation is useful in identifying the potential dynamic performance of the supply chain as a function of different operating policies, ahead of actual implementation of any one policy. In most cases, the simulations are stochastic in that they repetitively sample from distributions of uncertain parameters to build up distributions of performance measures.

As stressed in §3.1.2, characteristic models are of utmost importance since they are the closest representation of reality and provide a way to find the root of uncertainties at any level. Therefore, characteristic models are the most appropriate method for designing a fundamental bioenergy supply chain network. However, simulation models can be used to study the detailed dynamic operation of a fixed configuration under operational uncertainty, and can be used to evaluate expected performance measures for the fixed configuration to a high level of accuracy.

It is now a fact that European countries, including the UK, should invest heavily in renewable energy and incorporate it into their energy portfolio. So far there have been a huge number of research articles written regarding the technical aspects of bioenergy. However, there is a gap in the current understanding of its possible socioeconomic effects once it is introduced to the energy market on a large scale. Identifying biofuel’s key possible effects on local economies and the global energy market would be a valuable step in supporting decision-making at different levels. Therefore, model-based simulations can have great significance for policy makers, as they can identify the potential socioeconomic effects of the bioenergy supply chain under different operating policies, ahead of actual implementation of any one policy.

3.3. Supply chain planning and scheduling

Supply chain planning starts immediately after designing an infrastructure network and considers a fixed infrastructure over a certain time period, usually up to 1 year, and seeks to find the best network configuration to respond to forecast supply and demand in an economically efficient manner. In most of the work to date, the focus of researchers has been on identifying the best way to design the best network configuration based on demand uncertainty. However, as discussed earlier, there is not going to be a huge variation in ethanol demand; the main problem will be the variation of biomass supply due to seasonality. Therefore, the main issue for bioenergy supply chain planning will be finding the best network configuration using different feedstocks throughout the year to meet constant demand.

At this stage of development, most of processes are designed for specific biomass types; it should be emphasized that for a bioenergy network to be economically efficient, bio refineries should be able to use different feedstocks with only minimum changes made to their overall process. For example, processes should be flexible enough so that different operating conditions (i.e. different residence time or temperature in a bioreactor) are enough to process different types of feedstock, and it is not necessary to change the overall process configuration. It should be possible to get the same result from different feedstocks in an economically feasible manner. To conclude, authors believe process intensification—developing processes that are more responsive to market needs while responding to changes in process parameters in seconds, rather than several minutes or hours—is essential to designing an efficient global bioenergy network.

4. CONCLUSIONS

Over the past few years there has been huge body of literature published addressing challenges for commercial bioenergy production ranging from feedstocks to processes and products. However, there is lack of methodology on how to incorporate all the available knowledge into one interconnected network to answer key supply chain questions holistically. Thus, in this work we have described the key challenges in modelling the bioenergy supply chain and then developed a framework and methodology to show how multi-scale modelling can pave the way to answer holistic supply chain questions, such as how to design fundamental bioenergy supply chain and
incorporate process models into supply chain models. The
important next steps involve modellers working alongside
scientists engaged in fundamental experimental work on
biomass production and conversion, ensuring that there is
a good fit between the needs of whole systems modelling
and the generation of empirical data.

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