Thermo-economic optimal design of lignocellulose biorefineries

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Abstract

Energy demand is projected to rise in the following decades due to population growth, and with fossil fuels being the biggest contributor to global warming and climate change, efforts need to be made to foster an environment where sustainability is assured for future generations. Lignocellulose biomass is one of the most available and underused biological raw material by man. In this context, this paper is based on the collaborative development of a computer-aided platform whose objective is to optimize lignocellulose conversion pathways to heat, power and bio-based products – considering thermoeconomical objectives. The scope of the present work provides the integration methodology for unit process technologies. A demonstration of the developed framework is provided considering different levels of available biomass inputs.

Key words: biorefinery, lignocellulose, master-slave optimization, evolutionary algorithm, MILP, Wood2Chem

1. Introduction

There is a high scientific, economic and social significance in optimizing biomass conversion pathways. From a scientific point of view, and according to several authors (Marquardt et al., 2010; Kamm & Kamm, 2004a; King, Inderwildi, & Williams, 2010) the optimal conversion of biomass through biorefineries into highly value added products, while minimizing waste generation and environmental impacts, is an essential and challenging task. The conversion of lignocellulose biomass has recently been gaining attention globally, with lignocellulose biorefineries being touted for success (Kamm et al, 2007), an apparent fact with all the research and development in recent years (Floudas et al, 2012). Although the development of non-food based biofuel (or second generation biofuel) is pushing this initiative, a lot of other equally suitable product alternatives exist (Zhang 2008), and are being considered in an economical and environmental point of view (Santiba et al, 2011).

Biomass can be used nowadays in a different range of important products and subsequent applications, namely: in industrial applications as sources of heat and/or power generation (via gas burning in engines or turbines); can be made into fuel additives for transportation with

methanol or as a fuel itself as biodiesel; can be converted into several bio-based products, usable in a wide array of different industries, etc. More examples are presented in Bozell et al (2007) and Werpy et al (2004).

With so many different products and applications, it becomes hard to identify the best conversion pathways for biomass. With profitability and environmental performance as objectives in mind, the aim of this work is to support the development of a computer aided process tool, utilizing optimization algorithms, to identify the best alternatives for the conversion of lignocellulose biomass. On the economic standpoint, equipment investment and operation costs will be looked at, as well as product and resources market prices to evaluate profitability.

This computer aided tool, or software framework, is part of larger plethora of work that is being developed by the *Laboratoire d'Energétique Industrielle* (LENI) at the *École Polytechnique Federale de Lausanne* (EPFL). This project is called the Wood2Chem which is a framework platform with the purpose of performing multi-scale process design to synthesize conversion chains of wood, especially lignocellulose feedstock, into marketable products and energy services (Maréchal & Hungerbühler 2012). It is currently being developed in a partnership between the Safety and Environmental Technology (S&ET) group in Eidgenössische Technische Hochschule Zürich (ETHZ) and the Industrial Energy Systems Laboratory (LENI) of École Polytechnique Fédérale de Lausanne (EPFL).

The purpose of this framework will be to serve as an advanced decision support platform by using process modeling, multi-objective optimization and process integration techniques. Moreover, it will allow the systematic generation and comparison of wood conversion chains based on thermo-economic and life cycle environmental impact assessment criteria. When comparing with conventional approaches based on predefined scenarios, this approach aims not only to solve the material flow synthesis problem but also the heat and power integration problem. The scope of the analysis will adopt a multi-scale approach that will allow the formulation of the problem with the appropriate level of detail in order to generate conversion chains while integrating the available process model details.

The objective of this work is to define a methodology for the integration of unit process models and define an initial approach to multi-objective optimization. The multi-objective optimization is done using a master-slave dynamic, with an evolutionary programming algorithm as the master and a mixed integer linear programming algorithm as the slave. This optimization is done in a platform called OSMOSE and it is capable of analyzing the thermo-economic and environmental optimum conversion pathways for lignocellulose biomass.

OSMOSE is an acronym for “OptimiSation Multi-Objectifs de Systemes Energetiques integres”. It is a platform for the study and design of complex integrated energy systems. The software is being developed in the LENI at EPFL, in Lausanne, Switzerland. The project was motivated by the need for a flexible and high performance research tool for the study and design of energy systems (Palazzi et al. 2010).

2. Literature Review

As written by Maréchal & Hungerbühler (2012), the biorefinery concept gathers several important and very diverse fields of research: biofuel production, process systems engineering, biomass chemistry, biochemistry, biotechnology, agronomy and environmental science. This highly interdisciplinary dimension of this concept brings difficult challenges in aggregating and developing an overview of the field (King et al. 2010). Adding to this, the enormous variety of pre-treatment, conversion and separation processes available for transformation of biomass makes it even harder to find an optimal conversion path (Kokossis & Yang 2010). Therefore the use of a systematic computer aided approach has become a necessity, as described by several authors (Dimian 2007; Kokossis & Yang 2010; Tay & Ng 2012; Jr et al. 2007), to explore all the possible conversion pathways from wood to chemicals and energy taking into account mass and energy integration, economic

potential, environmental impacts, resource availability and corresponding supply chains. Kokossis & Yang (2010) highlights and discusses the role of systems technology to foster innovation, support computational experimentation and how it can be useful to complex and large problems typically found in chemical industrial facilities.

Gassner & Maréchal, (2007), define the methodology for the optimal conceptual design of thermochemical fuel production processes from biomass. The methodology described therein in decomposing of the problem in several parts is the concept behind using the master-slave optimization in the present work. Gerber et al, (2012a), in her extensive research of energy conversion systems in urban areas, further develops this concept for the computational framework and optimization problem – especially in defining the objectives to be used. The present work also relies on optimizations done in the past at LENI (Fazlollahi et al. 2012; and Fazlollahi & Maréchal, (2013).

The innovative part of this work, from the optimization angle, is to adapt these methodologies, which have so far been applied to the optimization of single unit processes, to several competitive and alternative unit processes. The concept of an optimum pathway is used to describe the desired solution from the optimization. However, since there are multiple objectives involved, there will be several optimum solutions, or several optimum pathways to consider. Thus, the results from the optimization will be provided, on the present work, in the form of a Pareto curve.

3. Methodology

The purpose of the Wood2Chem platform is to model the production design of a lignocellulose biorefinery and select optimum production pathways according to external conditions and objective criteria. This purpose is translated into an optimization problem which considers the unit process model data as parameters and unit model capacity sizing as variables. The major scope of the present work within the Wood2Chem project is the development of a unit process characterization methodology. This methodology is fundamental for providing the parameter data of the framework optimization. A preliminary optimization framework is also developed.

3.1. Computational framework

The computational framework in use builds from the works of Gassner and Maréchal (2009) and Gerber et al, (2012a). The framework in use is part of the OSMOSE platform and operates under Matlab. The methodology addresses the optimal thermo-economic process design for thermochemical fuel production from biomass characterized by an optimization problem, whose purpose is to choose different pathways that minimize simultaneously the costs and maximize the thermodynamic efficiencies. This is by essence a Mixed Integer Non-Linear Programming (MINLP) multi-objective optimization (MOO) problem. It is solved following a two-stage decomposition methodology where a master problem and a slave sub-problem are defined.

Figure 1 represents the overall computational framework built under OSMOSE where the Master and Slave optimizations are depicted. The unit process characterization developed in this work and its methodology is essential to provide the process parameters used in the Slave optimization. The framework has three main stages, the master optimization, the unit process characterization and the slave optimization, processing in that order with a cyclic nature.

The master optimization generates an initial group of pathways from a given set of decision variables – demand and price. The price variables are used in the unit process characterization methodology to select between different unit process configurations. The parameter data from the characterization methodology and the demand variables are then used by the slave optimization. The demand variables are used in the slave optimization for calculating the optimum pathway according to overall cost. These results are then sent back to the master optimization, and the master optimization selects the best, eliminates the weakest, and “breeds” a new population of improved pathways and the cycle repeats itself. As this is

an iterative process, it stops when a convergence threshold is reached.

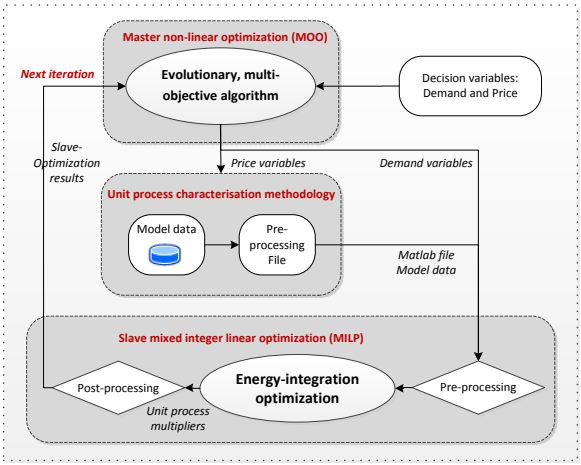

Figure 1 - Optimization framework implemented in OSMOSE

3.2. Unit process characterization methodology

The search for the optimum pathway is done by comparing the results amongst several alternative unit process models. These unit process models were built by several PhD students in the Wood2Chem project. Some examples include the works of Gerber et al. (2012), Gerber et al. (2011) and Peduzzi et al. (2013).

These unit processes were previously optimized, according to different technological configurations, product outcome, and other specific factors. The availability of unit process data is in the form of optimization results, namely Pareto fronts similar to the outcome this framework. This method integrates the unit process data in the framework as parameter data for the framework optimization. The important aspect is the flexibility of this method, which can later be adapted to suit various needs or changed/improved depending on future demands.

The major challenge of this methodology lay in the fact that the optimization framework only allowed one state or one set of conditions to define a unit process. For unit process data given in Pareto fronts, where each point had a distinct state and configuration, this proved problematic, because all the data needed to be included in the framework optimization.

The reasoning of this methodology is to evaluate all the points in a curve or several sets of curves, to find the best candidate to represent the unit process – according to a single predefined criterion. That criterion, chosen to leverage efficiency and cost, is the economic breakeven. To avoid creating a static best point from the rich selection of data, price variables from the master are used for degrees of freedom.

There are 3 main steps that compose the unit process characterization methodology: data extraction, cost recalculation and best point selection. The overall schematic is shown in Figure 2.

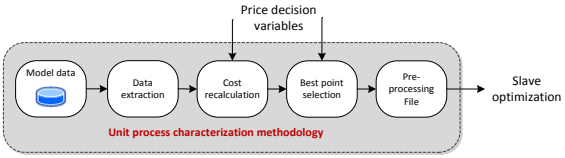

Figure 2 - Unit process characterization methodology

The first step of the methodology is extracting the information from the unit process data. Then a recalculation is done on the cost data for update. Afterwards a best point is selected, according to the economic breakeven. Following that, the information is stored in a pre-processing file used in the slave optimization.

3.2.1. Data Extraction

In a unit process model with data given in Pareto points, every point has several internal parameters defined, such as how much the input/output was or what was the cost. But it also has all the associated thermodynamic information of the process: the thermodynamic efficiencies, the temperatures, pressures, quality of streams, lower heating values of streams, etc. These internal parameters are also called *tags*. As the optimization only requires the frontier data of the model, its correct definition must first be undertaken and only the frontier description is taken into account.

3.2.2. Cost recalculations

A cost recalculation is necessary to update the values, to account for the changing economic conditions. The recalculation is done for the

operating costs, which encompass all the input materials for the unit process model. They are comprised of labor, maintenance, lignocellulose and electricity costs, but can change depending on the model specificities. To complement these calculations, the yearly costs and the cost per kWh are also updated.

3.2.3. Best point selection

The best point evaluation is done through the use of the economic breakeven calculation (Equation (1)). The selection is done with the point having the highest breakeven.

$$Breakeven\ (kW) = \frac{Annualized\ investment\ cost\ (USD/year)}{Output\ product\ price\ (USD/kWh)\ -\ Variable\ cost\ (USD/kWh)} \times \frac{1}{Year\ hours\ *\ 0{,}9} \quad (1)$$

Breakeven provides an evaluation considering operating and production cost (as variable costs), the investment cost, the interest rate and lifetime (in the annualized investment cost) and the product price (as a degree of freedom). This is the reason why this evaluation criterion was selected for comparison between the various points.

Afterwards, the data from the unit process Pareto point selected is used to generate the unit process parameters that will be sent to the slave optimization. These operations are compiled in a Matlab file and used as a pre-processing file in the slave optimization.

The integration of the Synthetic Natural Gas (SNG) database, created by Gassner & Maréchal, (2009) is one of the applications of this methodology. The unit processes in the Wood2Chem project are also developed in this manner, so this working methodology will also serve in their integration.

The SNG database has *circa* 124 different configurations, each a Pareto curve, each curve containing from 70 to 90 points and each with over 500 tags of information (reminder – tags are internal parameters of unit processes). The challenge was to include all these points for the optimization. The possible configurations were separated into 4 main groups: the circulating fluidized bed with oxygen feed (CFBO2); the fast internally circulating fluidized bed (FICFB); the pressurized fast internally circulating fluidized bed (pFICFB); and the pressurized fast internally circulating fluidized bed with a gas turbine (pFICFBgt).

4. Framework Application

A practical application for the platform was developed to showcase the results of the integration methodology and framework. This pathway optimization considers several levels of available biomass and analyses the subsequent optimal production results.

The main parameters that must be provided are the available lignocellulosic biomass and the decision variables. For the purposes of this application, the following range of input biomass was considered: 1, 5, 10, 20, 40 and 80 MW of Lignocellulosic biomass. The decision variables set for the optimization are divided in two main categories, price variables and demand variables. The demand variables, defined in megawatt are set to vary between 0 and the input lignocellulosic biomass – Table 1. The price variables, defined in US Dollar per megawatt hour, are set to vary between 10 and 200 [1] – Table 2. The definition of other optimization parameters is given in Table 3.

Each optimization was done considering total cost and total energetic efficiency objectives as previously defined in the post-processing section. The initial population size was set to 100 and 5000 was the maximum number of evaluations.

The optimization was realized on the EPFL's Bellatrix cluster, which is a Sandy Bridge based cluster available to the EPFL community since January 1st, 2013. The cluster is composed by[2] 424 compute nodes, each with 2 Sandy Bridge processors running at 2.2 GHz, with 8 cores each and 32 GB of RAM, for a total of 6784 cores.

[1] The electricity price, viewed at http://swissgrid.ch on the 6th of July 2013 was 14,53 cents USD/kWh; Synthetic Natural Price, viewed at http://epp.eurostat.ec.europa.eu on the 15th of June 2013 was 5,32 cents USD/kWh; Methanol, viewed at http://emsh-ngtech.com on the 15th June 2013 was 9,1 USD/kWh.

[2] Check source material for further hardware and server architecture information - http://scitas.epfl.ch/resources/bellatrix/

4.1. Results

The following graphs represent the various Pareto curves, the optimum productions (demand variables) and price variables for electricity and synthetic natural gas (Figure 3 to Figure 6). The following section provides an analysis of this data.

Table 1 – Demand decision variables

Variable	Interval (MW)
Electricity	[0 ; Input Biomass]
Synthetic Natural Gas	[0 ; Input Biomass]
Methanol	[0 ; Input Biomass]
Fischer-Tropsch fuels	[0 ; Input Biomass]

Table 2 – Price decision variables

Variable	Interval (USD/MWh)
Electricity bought	[10 ; 200]
Electricity produced	[10 ; 200]
Synthetic Natural Gas	[10 ; 200]
Methanol	[10 ; 200]

Table 3 - Additional parameters

Variable	Value
Marshall and Swift Index[3]	1536.5
Interest rate[4]	6%
Discount period	20 years
Plant availability[5]	90 %
Operators[6]	4 p/shift
Operator salary[7]	60'000 USD/year
Maintenance costs	5%/year of Capital cost
Biomass price[8]	65 USD/MWh
Biodiesel price[9]	126 USD/MWh
Maximum multiplication factor[10]	200

[3] Retrieved for 2012
[4] Interest rate and discount period: estimates from LENI, based on previous works.
[5] Plant availability refers to the yearly hours that the plant is considered to be functioning, meaning ninety percent of the 8760 total yearly hours. Source: estimate from LENI, based on previous works.
[6] Full time operation requires three shifts per day. With a working time of five days per week and 48 weeks per year, one operator per shift corresponds to 4,56 employees. For a plant size of 20 MW; Source: estimate from LENI, based on previous works.
[7] Source: estimate from LENI, based on average Swiss salary.
[8] Source: biomassenergycentre.org.uk accessed on the 5th June 2013.
[9] Source: http://www.extension.iastate.edu accessed on the 14th June 2013.
[10] The maximum multiplication factor defines the size each process unit can have above its sizing definition. It is an upper limiting scaling factor. It was set purposefully high so it won't be considered a limiting factor when considering the optimal pathway calculation.

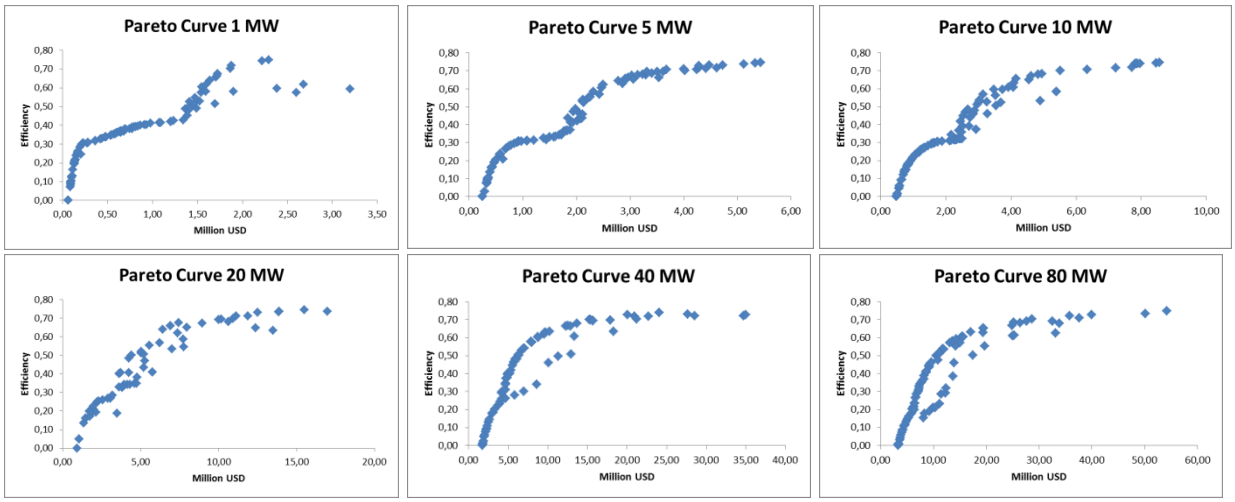

Figure 3 - Pareto curves for 1, 5, 10, 20, 40 and 80 MW

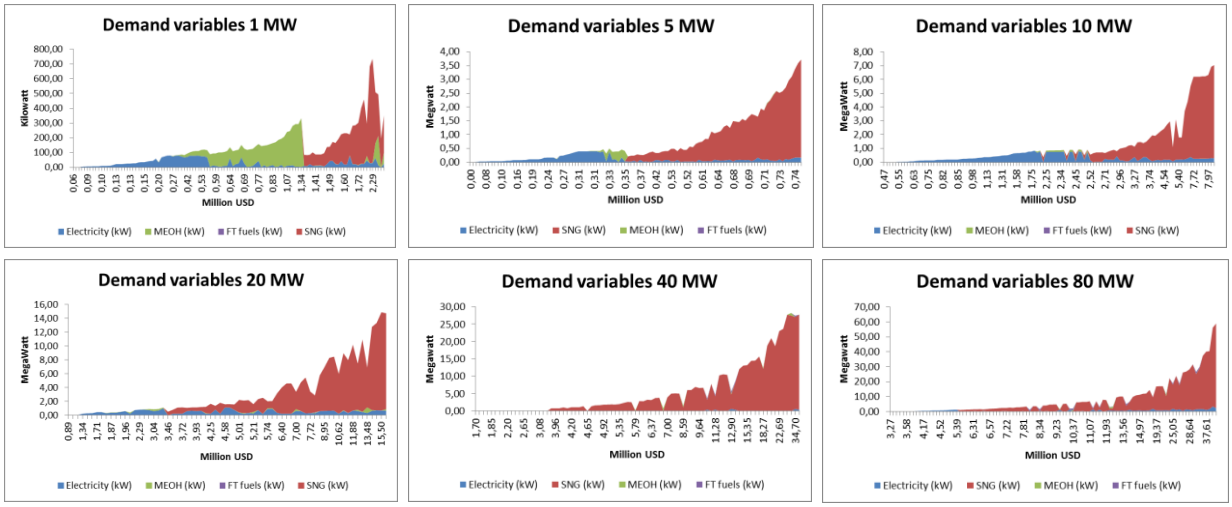

Figure 4 - Demand variables for 1, 5, 10, 20, 40 and 80 MW

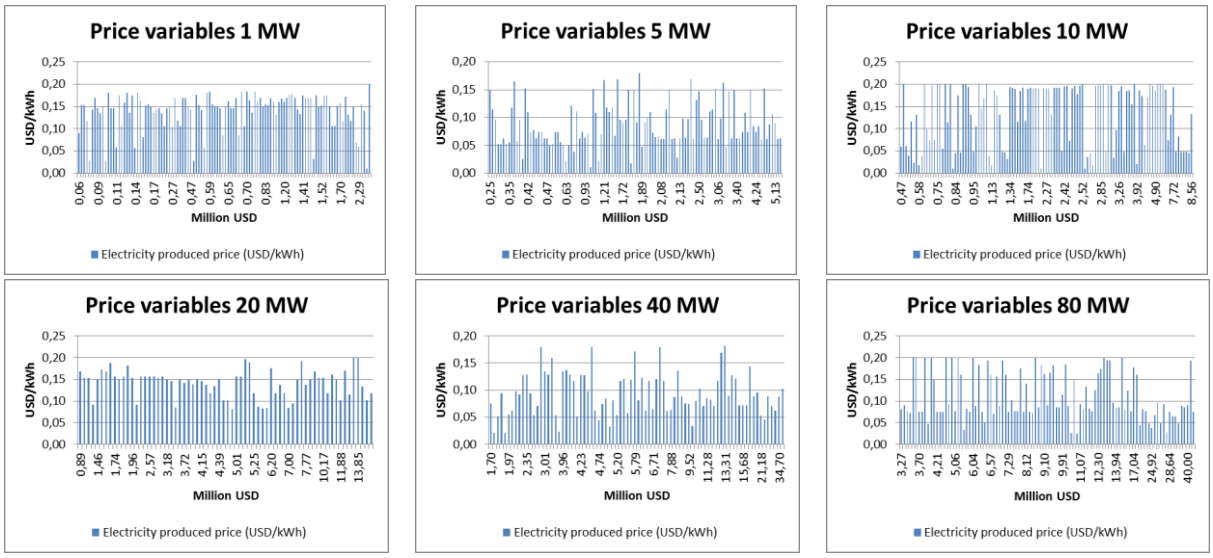

Figure 5 - Electricity price variables for 1, 5, 10, 20, 40 and 80 MW

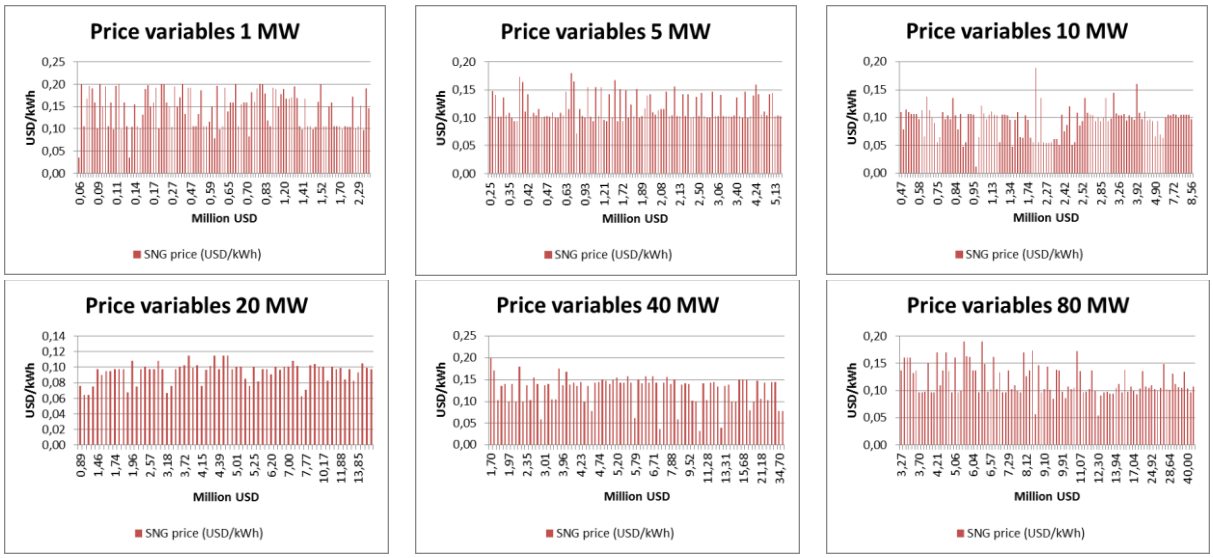

Figure 6 - Synthetic Natural Gas for 1, 5, 10, 20, 40 and 80 MW

4.2. Analysis

Regarding the Pareto curves, there are two noticeable features: an initial stratification of the curves becoming more uniform as the scale increases; and not all points reached are the optimal state. The stratification arises from the different alternatives in optimal productions which become apparent when looking at the demand variables results. The fact that not all points reached the optimum means that more iterations are required to reach the optimum.

The demand variables results clearly present a high preference for producing synthetic natural gas over the other alternatives. The Fischer Tropsch fuels are rarely chosen, and electricity and methanol are only optimal for very low scales.

There are many configurations / alternatives for synthetic natural gas than there are of the other models, this creates a vastly larger choice array for SNG solutions. It is then far likelier that better alternatives are present in SNG and better than the other solutions. Another aspect to consider is that the efficiency of the electricity and MeOH models are inferior to the SNG's, which allows efficiencies up to 75 per cent. Only in very small scale they are preferable, due to the SNG's cost scaling to those levels. On the other hand, the FT fuels model is very capital intensive when compared to the synthetic natural gas and methanol, reason why it is usually overlooked. The amounts of electricity being produced are co-products of the SNG process, and not the gas turbine or engine.

The price variables were expected to give an indication of the internal cost price of the technologies, and that they would decrease as the scale would go up, which is not what is verified. The first observation of prices is a lack of a clear trend. This might be occurring because they were not configured to be directly linked to the objectives – they neither influence the cost nor the efficiency objectives. Their influence is to alternate between configuration choices in the unit process characterization methodology – through the use of breakeven. Because of this, they may not be improving to an optimum as initially expected. Although some trends may be extracted for the prices, further work needs to be developed in analyzing the effects they are having in the optimization before attributing significance to their behavior.

Overall, the lack of interesting results comes from the limited number of unit processes modeled, with SNG being the favorite choice. On the prices side, the expected trend was not verified, due to it not being directly tied to the optimization's objective criteria. On the other hand, it is clear that the integration

methodology is doing its work, and that the synthetic natural gas model is exploring the alternative configurations in its database.

5. Conclusion

The purpose of this work was to improve the development of the Wood2Chem platform. The present work focuses on the development of a unit process characterization methodology and an optimization framework. The application of the optimization demonstrated the effectiveness of the methodology and the framework's capabilities.

The optimization framework consists of a two stage master-slave optimization, with the unit process characterization methodology bridging them. This developed methodology consists of a three stage process: data extraction, cost recalculation and best point selection. A case study, using the processes of SNG, Methanol, FT fuels and electricity was tested and the results were interpreted. The results showed a major preference for the SNG process as being the least costly and most efficient. This was due to the large number of SNG configurations available and their higher efficiencies.

There are several future possibilities and developments for this work. Integer cut constraints to list the best ranked pathways is already developed as of the first semester of 2014, as well as some initial thrusts into an overall superstructure. There is also considerable research being developed in analyzing succinic acid alternatives from lignocellulose as it has a relatively higher potential on the revenue side.

Further improvements of the framework may lie in the logistic side of the things, since it becomes complementary to the processual work being developed. Azcue (2013) developed a comprehensive model for the supply chain optimization of residual forestry biomass for Portugal. According to his optimization model, the operational costs of the biomass power plants were taken as a heuristic, considering the examples of other power plants in the country. The present work can take that model a little farther and provide more accurate and not only scalable costs, internal process-related information, but also other alternative products that could, in theory be produced.

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