

A two-level model to assess the economic feasibility of renewable urea production from agricultural waste

Diego C. Lopes^a, Moisés Teles dos Santos^a

^a University of São Paulo, Department of Chemical Engineering, São Paulo, SP, Brazil

* Corresponding Author: dclopes@usp.br

ABSTRACT

This work proposes a two-level model, combining process and supply chain models, and an optimization framework for an integrated biorefinery system to convert agricultural residues into renewable urea via gasification routes. The process model of the gasification, ammonia and urea synthesis was developed in Aspen Plus® to identify key performance indicators such as energy consumption and relative yields for urea for different biomasses and operating conditions; then, these key process data were used in a mixed-integer linear programming (MILP) model, designed to identify the optimal combination of energy source, technological route of urea production and plant location that maximizes the net present value of the system. The model was applied to the whole Brazilian territory, divided into 5569 cities and 558 micro-regions. Each region's agricultural production was evaluated to estimate biomass supply and urea demand. The Assis microregion, in close proximity with sugarcane and soybean crops, was found to be an optimal location for the plant, with an NPV of 110 MMUSD. Urea demand was found to be the main limiting factor, with more than 30 microregions needed to consume the plant's production. The results indicate the feasibility of producing renewable urea from agricultural waste and the importance of considering a two-level approach to assess the economic performance of the entire system.

Keywords: fertilizer, renewability, optimization

INTRODUCTION

Since 1961, worldwide food supply per capita has raised by 30%, in large part because of the increase of use of nitrogen fertilizers to improve agricultural productivity [1]. The importance of fertilizers on agriculture cannot be overstated, with research indicating that half of the world's population is sustained by mineral fertilizers [2]. Fertilizers account for a fifth of the producer's costs on the US [3], while on Brazil, the financial impact on cultures such as soya is between 30% and 40% [4]. The agricultural sector is also responsible for approximately 11% and 15% of all greenhouse gas (GHG) emissions worldwide [5], with fertilizers accounting for 2% to 3% of emissions [6]. Production of mineral fertilizers is dependent on fossil fuels and raw materials, including mineral extraction, transportation, manufacturing, and power supply. In this scenario, decarbonizing the fertilizer sector is equally important to the industry's expansion [7],

considering the GHG emissions reduction preconized in the 2015 Paris agreement.

The mineral fertilizers divide themselves into three main categories, each one corresponding to the main macronutrient present in its composition: nitrogen (N), phosphorus (P) and potassium (K). Although none of the macronutrients can be considered more or less important than the other, nitrogen is the one consumed at higher volumes, and also the one with the more energetically intensive manufacturing process and heavily reliant on fossil fuels throughout its manufacturing process, both as energy input and as a direct feedstock [2]. Out of all nitrogen fertilizers, urea is the main commercial product, produced by the synthesis of ammonia with carbon dioxide via the Basarov reaction [8]. Since both ammonia and urea synthesis are energetically intensive, efforts were made throughout the 20th century to improve its energy efficiency, involving equipment changes, process control and residual heat utilization. With these efforts, current

ammonia production is very close to the theoretical minimum energy consumption [2]. Considering the small efficiency improvements still possible, a natural future step is to search for sustainable replacements for the process' feedstocks and energy usages.

In this scenario, biomass is a promising feedstock replacement. Although biomass presents a polymeric structure, divided in cellulose, hemicellulose and lignin as its main polymers, it can be represented in a simplified way as a mixture of carbon (C), hydrogen (H), oxygen (O) and nitrogen (N) [9]. Most of the chemicals produced with oil or natural gas can be produced with biomass, by resorting to either thermochemical routes such as gasification or pyrolysis, or biological routes such as fermentation [10].

Urea production using biomass gasification as a feedstock has also been the object of recent studies [11-13] focused on process modeling and obtaining ideal operational parameters and technological routes. There is an obvious synergy in producing urea with agricultural waste, as the regions with high biomass supplies will necessarily have high urea demand. However, none of these studies consider supply-chain and location specific aspects, which can be critical at the planning stage [14]. This highlights the need to combine both a traditional process modeling approach with a robust optimization framework that takes spatial data, local biomass supply and urea demand into account. The present work proposes such a model to fill this literature gap.

METHODOLOGY

Process models

A process model of the full biomass gasification, ammonia and urea synthesis was developed in Aspen Plus v8.8 [13]. A simplified process topology is presented on Figure 1.

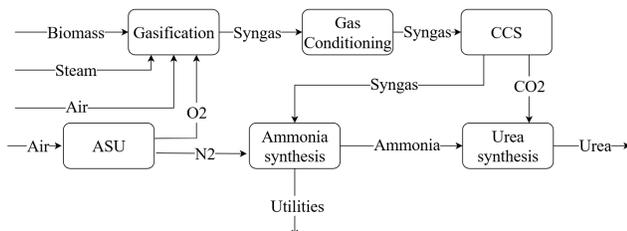
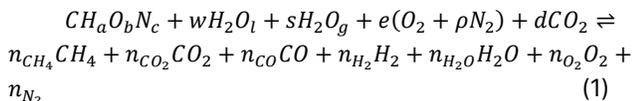


Figure 1. Process flow diagram

Biomass is firstly dried to 15% moisture and sent to a gasification unit, modeled with a non-stoichiometric equilibrium approach [15]. A global gasification reaction can be described as:



With a, b and c being derived from the biomass composition; w, s, e, ρ and d representing the gasifying agent mixture, and n being the number of moles of each component in the syngas. At equilibrium, the Gibbs energy of the mixture (G) must be at minimum:

$$G = \sum_{i=1}^M n_i G_i^0 + \sum_{i=1}^M n_i RT \ln\left(\frac{n_i}{n_{tot}}\right) \quad (2)$$

The number of moles of each component, n_i , are constrained by the mole balance of each atom C, H, O and N on the biomass. Tar formation is not considered in this model. The minimization of Gibbs energy is obtained on the Gibbs reactor block (RGibbs) in Aspen Plus. Syngas properties were calculated using the Peng-Robinson equation of state, with Boston-Mathias modifications.

The gasification agents are a mixture of air, steam and pure oxygen, produced in an air separation unit (ASU), with an optional CO_2 intake. The syngas composition is adjusted to improve H_2 concentration in a gas conditioning unit, consisting of two water-gas shift reactors and a methanation unit. The CO_2 present in the syngas is captured at a physical solvent carbon capture unit using DEPG (Dimethyl Ether of Polyethylene Glycol) as a solvent [16]. The purified syngas is mixed with nitrogen and sent to an ammonia synthesis unit, modeled with three catalytic beds and intermediate intercooling, based on a state of the art design [17]. The ammonia and captured CO_2 are sent to the urea synthesis plant, modeled as a CO_2 stripping process based on the commercial Stamicarbon® technology [8]. The final urea is concentrated to 99 wt. % in a double effect evaporator and sent to a granulation or prilling unit. A utility plant was designed to recover heat from the gasification, ammonia and urea synthesis. High pressure steam is generated in the syngas cooling stages and expanded into a multi-stage turbine to be used by the main steam consumers of the plant. The remaining steam generated is condensed at 0.1 bar, generating power. The purpose of the process model was to obtain the conversion of biomass to urea and the utilities consumption for any combination of operational parameters.

Supply-chain

The whole Brazilian territory was divided into 5569 cities, grouped in 558 micro-regions and 137 macro-regions. The open database PAM [18] from IBGE (Instituto Brasileiro de Geografia e Estatística) was used to obtain the total agricultural production for each location. Based on this, 5 crops were chosen as the most representative of the Brazilian agricultural scenario. Each crop's residue production was estimated using fixed ratios [19] to obtain an individual biomass supply for each location. Individual urea demand was also estimated using published data for mineral fertilizer usage by crop [20] and planted area.

Table 1 summarizes the chosen crops, biomass it produces and urea demand.

Table 1: Biomass supply and urea demand per crop

Crop	Biomass production (kg/ kg crop)	Urea demand (kg N / ha)
Rice	0.620	83
Coffee	0.295	161
Corn	0.672	68
Soy	0.690	16
Sugarcane	0.185	76

Sugarcane residue production is divided between straw and bagasse. Distances and travel times between all locations were obtained from geographical data [21]. Power prices were also individually considered using published tariffs [22].

Economical model

The capital costs for all subunits of the process were estimated by using the scale factor methodology [23], with an estimation of 368.7 MMUSD for a reference 35 t/h process. The CAPEX for other capacities ranging from 0 to 80 t/h was estimated using piecewise linearization.

Net present value is defined as:

$$NPV = \sum_{t=1}^n \frac{F_t}{(1+r)^t} - CAPEX \quad (3)$$

With F_t being the net cash flow at year t , r being the discount rate (by default at 10%) and $CAPEX$ being the total capital costs of the plant. Net cash flow is defined as:

$$F_t = -CAPEX_t + R + C_b + C_{tb} + C_{tu} + C_u \quad (4)$$

With R being urea revenue, C_b being biomass costs, C_{tb} being biomass transport costs, C_{tu} being urea transport costs, and C_u being utility costs.

Table 2 summarizes the main economical assumptions for the model.

Table 2: Economical assumptions

Parameter	Unit	Value
Urea price	USD/t	310.0
Biomass price	USD/GJ	4.50
Transport price	USD/km/t	0.058

Power prices are considered in a city-by-city basis using published tariffs.

Optimization model

A mixed-integer linear programming (MILP) optimization model was built using the Pyomo open-source software suite, to obtain the ideal location and capacity of a renewable urea plant, based on the process model performance. The model can be divided into 4 layers,

best represented in Fig. 2.

The model consists of 3 main sets:

L : set of possible locations (l)

B : set of biomasses (b)

R : set of technological routes for urea production (e.g.: pure oxygen gasification vs. air mixed gasification).

With:

CV_{br} : conversion of biomass b to urea at route r , in t urea/ t biomass

D_l : urea demand at location l .

S_{bl} : Supply of biomass b at location l .

The decision variables of the model are:

W_l : binary variable corresponding to the installation of the plant at location l

$BS_{bl'l'}$: biomass b sold from location l to location l'

BU_{brl} : biomass b used to produce urea via route r at location l

UP_{rl} : urea produced via route r at location l

$US_{ll'}$: urea sold from location l to location l'

C : capacity of the plant in tons urea/h

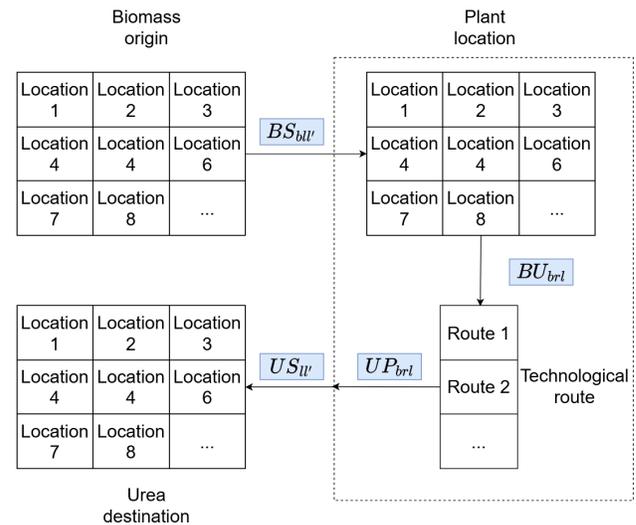


Figure 2 – Layers of decision

The objective function of the model is to maximize the NPV of the plant. Biomass consumption and utility usage for each technological route is given by the process model. Transport costs are calculated by using the distance from location l to location l' . The main constraints of the model, connecting the decision variables, are:

$$\sum_{l \in L} W_l = 1 \quad (5)$$

$$\sum_{b \in B} \sum_{r \in R} \sum_{l \in L} UP_{brl} = C \cdot 8300 \quad (6)$$

$$\sum_{r \in R} UP_{rl} = \sum_{l' \in L} US_{ll'} \quad \forall l \in L \quad (7)$$

$$\sum_{r \in R} UP_{rl} = M \cdot W_l \quad \forall l \in L \quad (8)$$

$$UP_{rl} = \sum_{b \in B} BU_{brl} \cdot CV_{br} \quad \forall r \in R, l \in L \quad (9)$$

$$\sum_{r \in R} BU_{brl} = \sum_{l' \in L} BS_{bl'l'} \quad \forall b \in B, l \in L \quad (10)$$

Table 3 – Process model results - Summary

Biomass	HHV (MJ/kg)	Moisture (%)	Route 1: O2 gasification		Route 2: Air mixed gasification	
			Conversion (t urea/t bio)	Utility (MWh/t bio)	Conversion (t urea/t bio)	Utility (MWh/t bio)
Rice husks	16.62	12	0.7015	0.3215	0.6894	0.2710
Coffee husks	20.92	12	0.8209	0.2716	0.7854	0.2356
Corn stover	19.06	15	0.7783	0.2905	0.7358	0.2487
Soy straw	18.53	15	0.7550	0.2971	0.7241	0.2513
Sugarcane straw	18.72	15	0.7616	0.2944	0.7211	0.2501
Sugarcane bagasse	18.16	40	0.5712	0.3261	0.5458	0.2771

Table 4 – Optimization model results - Summary

	Unit	Scenarios					
		Brazil	South	Midwest	North	Northeast	Northeast – Max.
Plant capacity	t/h	80.0	80.0	80.0	2.011	2.863	80.0
Total revenue	MMUSD	205.84	205.84	205.84	2.018	7.367	205.84
Biomass costs	MMSUD	62.078	61.773	61.793	1.458	1.983	62.433
Power costs	MMUSD	25.546	24.736	25.696	0.586	0.875	20.601
Biomass transport costs	MMUSD	5.049	5.476	5.040	0.132	0.184	6.522
Urea transport costs	MMUSD	9.593	10.737	11.018	0.096	0.202	36.309
FCF	MMUSD	103.572	103.115	102.29	2.901	4.122	79.970
CAPEX	MMUSD	772.29	772.29	772.29	23.94	34.075	772.29
NPV	MMUSD	109.476	105.592	98.569	0.764	1.018	-91.448

$$\sum_{l' \in L} BS_{bl'l'} \leq S_{bl} \quad \forall b \in B, l \in L \quad (11)$$

$$\sum_{l' \in L} US_{l'l} \leq D_l \quad \forall l \in L \quad (12)$$

RESULTS

Process model

The plant's performance was evaluated using the process model for all 6 types of biomasses and 2 technological routes, totaling 14 runs. Gasification temperature was set to 1200 °C, controlled by the oxygen intake. Two technological routes were chosen for this study: pure oxygen gasification, and air mixed gasification. In pure oxygen gasification, the only gasifying agent used is oxygen, while the nitrogen required by the ammonia synthesis is separated at the air separation unit and directly mixed before the syngas compression stage, controlling the N_2/H_2 ratio in the ammonia synthesis at 3.0. Meanwhile, in air mixed gasification, the air intake controls the N_2/H_2 ratio and oxygen is complemented to keep the gasification temperature at the desired setpoint. Table 3 summarizes the results. The informed utility consumption already takes into account internal power production; overall, oxygen gasification is more efficient in converting

biomass into urea, but power generation is also smaller in comparison. Sugarcane bagasse has high average moisture, which explains the large difference between this biomass and all the others. Also, higher moisture increases steam consumption in the drying stage but reduces the need of steam injection at the gas conditioning phase to adjust the gas composition.

Optimization model

The commercial solver Gurobi was used to solve the MILP model, taking 19.11 mins on average on a Ryzen 7 CPU at the largest simulation. The database used in the simulations, as well as the full results, are provided in the supplementary material. Table 4 provides the summary of the results.

The optimization model was initially applied to the whole country at the micro-region level (558 locations). In this scenario, it was found that the Assis microregion in the state of São Paulo is the optimal location for the installation of the renewable urea plant. Pure oxygen gasification was the route chosen, and the biomasses used are a 50/50 mix of soybean straw and sugarcane straw, leveraging the large sugarcane crops in the São Paulo state. The plant capacity was constrained to a maximum

of 80 t/h to limit the errors on capital costs estimation. The total urea produced (663,000 tons/year) is enough to supply 50% of the state demand and 9.2% of the national urea demand.

The Assis microregion has enough biomass available to provide 99% of the required biomass of the plant. However, the urea produced needs to be sold 30 different microregions, crossing state borders and navigating more than 250 km. Figure 4 shows the plant location and all optimal markets for the urea product destination.

The model was constrained to other regions of Brazil to evaluate local feasibility. In the south region, the microregion of Cianorte presented the best NPV results, using a mixture of rice husks and sugarcane straw as biomasses. In this case, the local supply of biomass is not enough to satisfy the plant's demands, so biomass needs to be imported from close regions, which raises transport costs. The Midwest region consists of a large agricultural belt in Brazil, and the optimal location in this region was found to be the "Sudoeste de Goiás" microregion. At this scenario the plant uses 100% soybean residues, which forms much of the biomass available in the Midwest. In both scenarios, the urea must also be sold to more than 20 locations as the local markets cannot accommodate the total plant production.

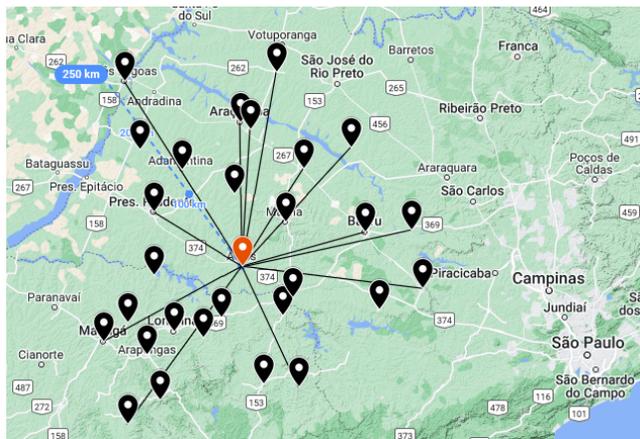


Figure 4 – Plant location and urea consumers for main scenario.

The model's results for the other two regions of Brazil (North and Northeast) show that a large-scale renewable urea plant is not feasible, with optimal capacities of 2.01 and 2.83 t/h respectively. Despite large biomass supplies in these regions, the distance between urea markets is too large and local urea demand is too small, to the point where the logistical costs of transporting urea become the main limiting factor. To illustrate this, an additional scenario, called "Northeast – Max." was modeled constraining the possible locations to the Northeast region but also fixing the plant's capacity to the maximum (80 t/h). In this scenario, the NPV is -91 MMUSD, with the

urea transport costs increasing to 36 MMUSD.

CONCLUSIONS

A two-level model for the production of renewable urea was developed, combining a traditional process model with a supply-chain and optimization framework. The process model was applied to 6 different biomasses and 2 technological routes, obtaining the key performance indicators (KPIs) for all 14 scenarios. These KPIs were used in the supply-chain model to obtain the optimal combination of plant location, biomass used and technological routes considering local biomass supplies, urea demands and distance between regions. It was found that the optimal location for a renewable plant in Brazil is in the São Paulo state, given the high urea demand and short distances between markets. When constraining the model to different regions, it was found that the logistical costs of urea distribution bottlenecks the feasibility of the plant. This highlights the need for a robust supply chain model coupled with a traditional process modeling approach.

DIGITAL SUPPLEMENTARY MATERIAL

The database used in the simulations, as well as the full results, are provided in the following link, hosted in the Living Archive for Process Systems Engineering – LAPSE: <https://psecommunity.org/LAPSE:2025.0015>

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