Whole-system Optimisation for Carbon Footprints Reduction of Corn Bioethanol

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Abstract: Whether biofuels production from starchy biomass can actually be environmentally is still an open question. A modelling approach for strategic systems design combining lifecycle analysis (LCA) and supply chain optimisation (SCO) analysis can significantly contribute to clarify the question. Here we discuss the possibility of managing and optimising the biomass cultivation stage and its integration through the entire production network in order to tune the environmental performance of bioethanol production. The design task is addressed through a quantitative modelling tool, which aims at steering crop management towards the best fertiliser usage and distillers dried grains with solubles (DDGS) end-use in order to ensure optimal whole system performance in terms of both profit and greenhouse gas (GHG) emissions.

Results shows how a crop management strategy devised from a whole systems perspective can significantly contribute to reduce biofuels carbon footprints. In particular, it is observed that through whole systems optimisation, the GHG emissions of so-called first-generation biofuels can approach those associated with second generation ones.

Keywords: Bioethanol, Whole system optimisation, Supply chain, GHG emissions

1. Introduction

Over the past years biofuels for transport have been acknowledged as one of the key issues within the world energy agenda. Among the alternatives, bioethanol through first generation productions was first hailed as the most appropriate solution aiming at a partial substitution of oil-based fuels. Although the initial verve, founded on the potential economic benefits as well as on the energy supply security ensured by a broad range of suitable feedstock (i.e sugar cane and starchy biomass), the first generation pathway has recently known oppositions by both the public opinion and part of the academic community. The core of the question revolves around ever increasing doubts on whether bioethanol could effectively ensure the expected potential in terms of global warming mitigation, particularly when the energy vector derives from the conversion of starchy biomass [1,2].

This did contribute to heat up an already existing debate on the actual carbon footprints of these productions. Most of the studies addressing the question [1-6] state that ethanol derived from starchy biomass can actually contribute to a partial oil displacement [3,4,6], although the effective environmental impact tightly relates to the technological and geographical context in which the system performs, and to specific details in the operation of the overall supply chain. For example, GHG emissions from corn-based ethanol production can be estimated between 3% and 86% [5] lower than the emissions from gasoline production, depending on how the ethanol is produced. This large variability is mainly related to biomass production conditions: climate, properties of soil, cropping management and cultivation practice in general [3] can generally contribute to about 45% of the overall GHG emissions [7]. The raw nerve is represented by mineral fertilisers (mainly nitrogen-based ones) as their extensive application in biomass cultivation stage is the primary source of GHG such as nitrous oxide (N₂O) [8]. On the other hand, nitrogen dosage would also entail *direct effects* on biomass production

parameters and, as a consequence, *indirect effects* on the subsequent stages of the network itself. Technically, increasing the nitrogen input per unit of cultivated land causes: *i.* a direct increase in the corn yield, and, indirectly, in the ethanol yield; *ii.* a direct increase in the yield of grain protein to the detriment of starch content of corn grains, and, indirectly, improving the by-products (i.e. DDGS) yield to the detriment of the ethanol yield; *iii.* a direct increase in costs related to fertilisers, but indirectly to reducing operating overheads as an indirect consequence of the potential increase in both ethanol and DDGS yield; *iv.* an indirect increase of the total global warming impact due to greater GHG emissions coming from both fertiliser production and N₂O release from soil.

Another important aspect of the lifecycle emissions relates to the end-use of valuable sub-products (e.g. heat and power or DDGS), and the assumptions about the products that they displace (e.g. coal-derived energy and soya meal) [7]. This is influenced by nitrogen application, too: the potential increase in by-products yield coming from the over-dosage of mineral fertiliser can cause an indirect increase in emission credits coming from products displacement.

All these issues evidence a conflicting situation which cannot be cleared up by means of a mere heuristic evaluation of the pros and cons of fertiliser application. Thus, it raises the obvious need for a fully integrated analysis embodying all those issues (i.e. global warming mitigation together with economic and financial feasibility) that may help defining a more comprehensive and quantitative view of the interactions along the entire biofuels production system so as to assist both crop and fuel producers and, most importantly, policy makers in their strategic decisions. To the best of our knowledge, no analysis has so far been presenting the adoption of modelling tools to *optimise* the overall bioethanol supply chain by taking into account the entire set of production stages in the supply chain including biomass cultivation.

Some of our prior works have addressed the development of optimisation tools linking LCA and SCO models (i.e. Multi-objective Mixed-Integer Linear Programming - MoMILP), and specifically devised for the optimisation of both the environmental and economic performance of biofuels production [7]. Here we discuss the possibility of managing and optimising the biomass cultivation stage, too, and its integration within a quantitative MoMILP model which aims at tuning the environmental performance of bioethanol production so as to identify strategies for deep, system-wide reductions of GHG emissions.

Eventually, the emerging biomass-based ethanol production in Italy is assessed as a real world case study to demonstrate the actual approach capabilities in steering the crop management toward the best overall nitrogen fertiliser usage and DDGS end-use technical choice ensuring best whole-system performance in terms of both profit and GHG emissions.

2. Methods and modelling assumptions

The modelling framework here described is conceived as an optimisation problem in which the production chain is required to comply with both profit maximisation and impact minimisation criteria. Key components of the optimisation problem include biomass production response to nitrogen dosage (yields, costs, etc); biofuel production facilities capital and operating costs as a function of biomass characteristics; transport logistics costs and emissions; environmental burdens of biomass and biofuel production as a function of nitrogen dosage as well as of the DDGS end-use options; and energy market features (energy purchase prices and green credits).

The objective is to determine the optimal system configuration in terms of financial profitability (NPV) and GHG emissions. Therefore, key variables to be optimised include nitrogen dosage over the biomass crop field, DDGS end-use solution, system financial performance over a 10 years horizon and system impact on global warming.

The problem is referred to a fixed land surface (30,000 ha) fully cultivated to supply the biomass needs of a unique production plant of flexible capacity, anyway ranging within a consistent interval, namely 80–120 kt/y.

2.1. Mathematical formulation

The mathematical formulation of the proposed framework is based on the modelling approaches adopted in the design of multi-echelon SCs [9,10], by also introducing multi-period features to address the financial analysis (which is performed over a 10-years time horizon).

2.1.1. Objective functions

The first objective considered is the NPV (Obj_{NPV} [€]) of the business to be established. This imposes the maximisation of profit-related indexes, and hence the Obj_{NPV} value is required to be written in its negative form:

$$Obj_{NPV} = -NPV = FCC - DNI \quad (1.a)$$

where FCC [€] are the facility capital costs and DNI [€] represents the discounted net incomes.

The second objective is to minimise the total daily GHG impact (Obj_{TDI} [kg CO₂-eq/d]) resulting from the SC operation. Thus, the definition of Obj_{TDI} needs to consider each life cycle stage contribution, as expressed by the following equation:

$$Obj_{TDI} = \sum_s I_s \quad (1.b)$$

where I_s [kg CO₂-eq/d] are the stage-related environmental impacts resulting from the operation of the single stage s .

2.1.2. Economics

The FCC term accounts for the capital investment required to establish a new fuel conversion facility. However, this model allows for the choice between two different technological options according to the two mentioned options proposed for DDGS use: $k = 1$, which involves the standard conversion technology in which DDGS is processed as a simple by-product to be sold to the animal fodder market; or $k = 2$ which envisages the construction of a CHP station fuelled by DDGS to produce heat and electricity.

According to this, FCC can be calculated by alternatively assigning the capital investment value (CI_k [€]) corresponding to the technological features adopted, as expressed by:

$$FCC = \sum_{n,k} CI_k \cdot W_{n,k} \quad (2)$$

where $W_{n,k}$ is the binary decision variable controlling whether to establish a production facility of type k when a nitrogen dosage n is applied: a value of 1 allows for the construction of the plant type k , otherwise 0 is assigned.

The discounted net incomes DNI is defined as the sum over the 10 year operating period of the annual profit before taxes (PBT [€/y]) plus the annual depreciation charge related to the capital investment (D [€/y]) minus the taxation charge for each year t (TAX [€/y]), as expressed by the following equation:

$$DNI = \sum_t (PBT - TAX + D) \cdot \varepsilon_t \quad (3)$$

All the terms on the right hand side of Eq. (3) have been discounted through the application of a discount factor (ε_t) defined as [11].

The profit before taxes PBT represents the gross annual profit and has been defined as the difference between the total annual revenues TAR [€/y] and the total operating costs OC [€/y] for year t minus the depreciation charge D . Accordingly:

$$PBT = TAR - OC - D \quad (4)$$

TAR represents the annual incomes which depend on both ethanol and DDGS sales:

$$TAR = MPe \cdot \sum_{n,k} Pe_{n,k} + \sum_{n,k} Pd_{n,k} \cdot MPd_{n,k} \cdot \omega_k \quad (5)$$

where MPe is the bioethanol market price (set equal to 709 €/t according to [12]); $Pe_{n,k}$ [t/y] and $Pd_{n,k}$ represent, respectively, the ethanol and DDGS production rate related to plant technology k when a nitrogen dosage n is applied to crop biomass; $MPd_{n,k}$ is the DDGS market value and depends on the DDGS end-use solution k . When DDGS is used as soy-meal substitute in the animal fodder market ($k = 1$), $MPd_{n,1}$ is the market price that also depends on the nitrogen dosage n . On the other hand, if power generation is chosen as the end-use option ($k = 2$), $MPd_{n,2}$ identifies the average market price per unit of electric energy sold to the grid. This does not depend on the nitrogen dosage n in any case. This modelling solution also requires the application of a conversion factor, $\omega_{n,k}$, to quantify the amount of by-product produced per unit of DDGS. Thus, when power generation is chosen as end-use solution ($k = 2$), $\omega_{n,2}$ [kWh_e/t_{10%DM}] identifies the amount of energy that can be sold to the grid per unit of DDGS produced. On the other hand, when DDGS is used as a soy-meal substitute in the animal feed market ($k = 1$), the amount of by-product to be sold should be equal to the overall DDGS production. In order to comply with Eq. (5), $\omega_{n,1}$ [t/t] has been set equal to 1.

OC is given by the sum of the annual operating costs over the entire supply chain. This has to account for the contribution of all the supply stages (s), i.e. biomass production (BP), ethanol and DDGS production (EP) and transports (for biomass, BT, and ethanol, ET), minus the by-products allocation credits (BC). Accordingly:

$$OC = \sum_{n,k} \left[(Pb_{n,k} \cdot UPCb_n)_{BP} + (Pe_{n,k} \cdot UPCE_n)_{EP} + (UTCb \cdot Pb_{n,k})_{BT} \right. \\ \left. + (UTCe \cdot Pe_{n,k})_{ET} - (Pe_{n,k} \cdot UCRd_{n,k})_B \right] \quad (6)$$

where $Pb_{n,k}$ represents the biomass production rate supplying a conversion plant of type k when a nitrogen dosage n is applied to crop fields, $UPCb_n$ [€/t_{DM}] and $UPCE_n$ [€/t] are respectively the unit production costs for biomass and ethanol, $UTCb$ [€/t_{DM}] and $UTCe$ [€/t] define the unit transport costs for biomass and ethanol respectively, and $UCRd_{n,k}$ is the cost reduction per unit of DDGS used as a valuable alternative k and produced when a nitrogen dosage n is applied.

The last factor defining *PBT* in Eq. (4) is the depreciation charge *D* evaluated by simply dividing the total capital investment (*FCC*) by 10 (thus assuming a constant depreciation strategy).

2.1.3. Environmental impact

The definition of stage-related environmental impacts I_s [kg CO₂-eq/d] resulting from the operation of the single stage *s* is calculated as follows:

$$I_s = \sum_{n,k} f_{s,n,k} \cdot F_{n,k} \quad \forall s \quad (7)$$

where $f_{s,n,k}$ is the global emission factor representing the carbon dioxide emissions equivalent at stage *s* for technology *k* and nitrogen dosage *n* per unit of reference flow; whereas $F_{n,k}$ uniquely defines the reference flows for each individual life cycle stage and expresses them explicitly as a function of the design variable controlling the optimisation problem. In this problem $Pb_{n,k}$ represents the reference flow for biomass production and biomass transport, $Pe_{n,k}$ for ethanol production and ethanol transport, whereas $Pd_{n,k}$ refers to the emissions credits.

2.1.4. Logical constraints and mass balances

All the variables defined in the above are linked to the specific SC features through the definition of a set of constraints that must be satisfied in each of the SC stages.

A set of relations is formulated to constrain the goods production rate together with the binary variables. In particular, $Pb_{n,k}$ is the dominant production variable and is defined as follows:

$$Pb_{n,k} = LA \cdot GY_n \cdot W_{n,k} \quad \forall n, k \quad (8)$$

where *LA* [ha] is the land availability (30,000 ha, as declared in the previous section) and GY_n [t_{DM}/ha] the grain yield per hectare when a nitrogen dosage *n* is applied.

Once the biomass production is quantified, the ethanol and DDGS production rates can be derived by simply applying a specific conversion factor. Accordingly:

$$Pe_{n,k} = Pb_{n,k} \cdot \gamma_n \quad \text{and} \quad Pd_{n,k} = Pb_{n,k} \cdot \delta_n \quad \forall n, k \quad (9)$$

where γ_n [t_{biofuel}/t_{biomass}] and δ_n [t_{10%DM}/t_{biomass}] are respectively the alcohol and DDGS yields when biomass is cropped by applying a nitrogen dosage *n*.

2.2. Response curves

The definition of the variables response to nitrogen dosage is based on the comprehensive work by Smith et al. [13], which, however, refers to wheat. Since no complete sets of data could be retrieved on corn, it was decided to tune up the wheat data set to corn cultivations on the few data available. Correlations for wheat reported in [13] have been used to define both the graphical and the mathematical dependence of corn grain yield (*GY*), grain protein content (*PY*), DDGS yield (*DDGSY*) and alcohol yield (*EY*) on nitrogen dosage (*ND*). The entire set of model parameters and their inherent dependence on nitrogen application have to be estimated on the basis of these response curves. Because we wish to maintain model linearity, we use a piecewise linear dependence of key variables on nitrogen dosage. The nitrogen dosage variable is discretised into a number (=12) of intervals *n* (25 kg_N/ha of extension). Note that in general climatic and land characteristics may have an impact on the actual crop

response to nitrogen dosage and this should be taken into account when applying the methodology.

The technological related parameters, i.e. GY_n , δ_n , γ_n and μ_n , have been directly obtained by the corresponding response functions. In particular, μ_n is the soy-meal replacement factor representing the amount of soy-meal that can be replaced by DDGS. Thus, in this work we do not assume an allocation by energy on DDGS, but a substitution as fodder at iso-nitrogenous and iso-energetic conditions. According to [14], this has involved the application of a substitution ratio of about 0.68 kg_{soy-meal}/kg_{DDGS} (defined assuming a DDGS protein content of about 76% compared to soy-meal). Then, the DDGS protein content (and, hence, the substitution ratio response to nitrogen) has been scaled according to the nitrogen dosage applied.

On the other hand, both economic and environmental parameters has been defined adapting the approaches of [7,15] by varying the nitrogen-dependent inputs according to the trend in the response curves.

3. Results and discussion

The modelling framework as presented was used to determine the optimal system configuration according to the two conflicting objectives discussed in the above. Design variables (the nitrogen dosage over the biomass crop field and the DDGS end-use option) were optimised by means of the CPLEX solver in the GAMS[®] modelling tool [16]. The model considers two technological options for DDGS end-use: *i*) soy-meal substitute to be sold in the animal fodder market, or *ii*) fuel fed to a combined heat and power (CHP) station. A first instance has been assessed by assuming standard market conditions for the electricity selling price ($MPd_{n,2} = 91.34$ €/MWh_e). The sub-optimal set of solutions (◆) coming from the trade-off between the environmental (total impact, TI, expressed in kt CO₂-eq) and the financial (Net Present Value, NPV, expressed in M€) criteria is reported in Fig. 1.

Fig. 1. Pareto set of solutions: NPV vs. Total Impact (TI)

Point A on the diagram represents the best optimum in terms of economic performance that can be obtained by applying a nitrogen dosage of 237.5 kg_N/ha and using DDGS as animal fodder substitute. However, this is not a feasible solution if we consider the EU targets (which impose a minimum of 50% of emission savings with respect to conventional fuels by 2017): point A, indeed, corresponds to a GHG emissions reduction of about 21% that totally amount to 238.9 kt CO₂-eq (about 67.6 kg CO₂-eq/GJ_{EIOH}). The mentioned target is never met if we

keep using the DDGS as animal feed substitute. Thus, it is worth to investigate on the other alternative, namely the use of DDGS to fuel a CHP station. In this case, we assist to a sensible GHG emissions reduction by still remaining within the economic feasibility region. It is possible to obtain payback times lower than 6 years from point B up to point C. The environmental optima (that also assures feasible economic conditions) involves a nitrogen dosage of 87.5 kg_N/ha (point B) so allowing for a GHG emissions reduction of about 80% (17.1 kg CO₂-eq/GJ_{EtOH}) with respect to gasoline and realising an NPV of about 25.7 M€ (the payback time is still reasonable and amounting to about 6 years). On the other hand, the financial optima (still assuring feasible environmental performance) involves a greater nitrogen dosage (162.5 kg_N/ha, point C) so resulting in higher GHG emissions, although still more than acceptable (21.2 kg CO₂-eq/GJ_{EtOH}, corresponding to 75% of emissions savings with respect to gasoline), and realises an NPV of about 38.5 M€ (the payback time is now 5.5 years).

The situation might be even more profitable if the bioethanol business would be supported by governmental subsidies, as it is actually envisaged according to the latest Italian regulation on renewable energy: accordingly the electric energy produced from renewable energy sources can be sold at a price of 180 €/MWh_e. The positive effect of these subsidies is evident from the set of sub-optimal solutions (Δ) reported in Fig. 1. Considering the solution involving DDGS as animal feed substitute, the situation does not change because green credits do not affect the financial features of this option. On the other hand, the financial performance is actually enhanced if DDGS is used to fuel a CHP station: the points between D and E represent feasible options in terms of both economic and environmental criteria. For instance, by applying a nitrogen dosage of 37.5 kg_N/ha (point D) the environmental optima entails a GHG emissions reduction amounting to about 82% (15.8 kg CO₂-eq/GJ_{EtOH}) with an economic profit of about 27 M€ over a 10 years horizon (the payback time is about 6 years, still). However, if the profit maximisation is preferred, it is possible to apply up to 162.5 kg_N/ha (point E) so as to keep within the environmental feasibility region (the GHG emissions reduction would be 75% with respect to gasoline) and realising excellent financial performance: as shown in Figure 7.6, the NPV now amounts to 68.4 M€ so allowing for the lowest payback time (4 years).

4. Conclusions

It is clear that the analysis of biofuels production is a complex task, particularly when environmental issues are taken into account. Broader information, analysis tools, interactions between different types of expertise are necessary to obtain a full comprehension of such a multifaceted problem. If the final goal is fuel instead of food, the overall chain might have to be operated in a different way and the boundary between “first-generation” and “second-generation” biofuels may start blurring. This is why decision makers should be provided with tools capable of evaluating how the system may react to different options and how its design may change if optimised towards specific goals. On the one side, it is important to identify the existing optimal points; on the other hand, we need to assess how flexible the system is in terms of profitability, GHG emissions and environmental and social impacts.

In this contribution we showed how whole-system optimisation tools can be exploited to address these issues. We considered the nitrogen balance optimisation and the technology selection in a first generation bioethanol supply chain according to economic and environmental goals. Results demonstrate that the only way to meet the EU standards (50% of GHG emission savings by 2017) on corn bioethanol in Italy is to adopt a technological solution envisaging the construction of a CHP station to be fuelled with DDGS. This requires

moderate nitrogen dosage as a mineral fertiliser (about 160 kg_N/ha) so as to reach GHG emission savings of about 75% with respect to gasoline production. It is also worth mentioning that a more thoughtful use of mineral fertiliser would also reduce other environmental impacts associated with fixed nitrogen application to agricultural soils (i.e. eutrophication and acidification of the ecosystem). However, this would require support through the deployment of governmental subsidies so as to ensure all the competitiveness and economic efficiency requirements imposed by the global market.

Over the years, the discussion has broadened by incorporating the analysis of the entire supply chain and more recently even the indirect effects of land use change. In fact, future work will need to deal the analysis and modelling of the effects that the land conversion from crop-for-food to crop-for-fuel would generate.

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