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Multi-Objective Optimisation in a Petrochemical Complex with LCA considerations

Antonio González-Castaño, J. Alberto Bandoni, M. Soledad Diaz*

Planta Piloto de Ingeniería Química (PLAPIQUI) CONICET-Universidad Nacional del Sur, Camino La Carrindanga Km 7, Bahía Blanca 8000, Argentina.
sdiaz@plapiqui.edu.ar

Abstract

In this work, we address the optimization of an entire petrochemical complex using economic and environmental criteria. The site mathematical model includes linear and non-linear simplified models for single plants to calculate site production, taking into account main operating variables, intermittent deliveries and inventory variable profiles. The environmental objective is measured with the global warming potential (GWP) and ReCiPe metrics according to the life cycle assessment procedures using indicators at two levels: eighteen midpoint indicators and three endpoint indicators realised in SimaPro (Pre-Consultants, 2015).The resulting mixed integer nonlinear programming (MINLP) models are implemented in GAMS. The bi-criteria MINLP model is solved with the ε-constraint method. Mid-point indicators are presented for current conditions. Numerical results show that the petrochemical complex can satisfy product demands while improving the environmental performance by decreasing greenhouse gases emissions in 33 %, from 1,042 to 695.33 kt CO_2-eq/year in the case of GWP minimization.

Keywords: Multi-Objective Optimisation, Life Cycle Assessment, Petrochemical Complex.

1. Introduction

During the last decades, much effort has been devoted to optimise petrochemical processes to improve energy integration and economic performance. To ensure sustainable production of petrochemical products, the inclusion of environmental targets within optimization objectives is mandatory. Environmental concerns are considered as part of the objective design and not as additional constrains in similar design process systems (Ciumei et al., 2004; Guillén-Gosálbez and Grossmann, 2009; Cortes-Borda et al., 2015). In this context, life cycle assessment (LCA) is a standard procedure to evaluate the environmental performance of a process. It calculates environmental loads associated to a product, a process or activities from raw material acquisition and others supplies required for the production to the final disposition of products (ISO-14040, 2015). Numerical results are presented as a set of environmental impacts that can be aggregated into different groups, eighteen mid-point impact categories are proposed (Goedkoop et al., 2013), which are further aggregated into three end-point indicators.

In this work, we perform multi-objective optimisation of an actual petrochemical complex, located in Argentina, considering both economic and environmental objectives. Previous work has included the economical optimisation of the entire complex (Schulz et al., 2005). The site includes two natural gas liquids (NGL) processing plants, two ethylene plants, a caustic soda and chlorine plant, a VCM plant, a PVC plant, three polyethylene plants (LDPE, HDPE, LLDPE), an ammonia and an urea plant. The objective functions are profit maximisation and environmental impact minimisation. Constraints include mass and energy balances, bounds on product demands, equipment capacities and intermediate and final product storage tanks limitations. There are also constraints on final products distribution by ship, train or truck while storage tanks capacities must be satisfied. The environmental objective is measured with the global warming potential (GWP) and ReCiPe metrics according to life cycle assessment procedures. The resulting problem is a mixed integer non-linear programming (MINLP) optimisation problem, implemented in GAMS (Brooke et al., 2015).

2. Process description

The petrochemical complex under study is the largest in Argentina. It comprises two natural gas processing plants, whose main objective is to extract ethane from natural gas to use it as raw material in ethylene plants. Natural Gas Plant I, next to the complex, is fed with 24 Mm^3/d of natural gas. Residual gas (mainly methane) is recompressed to pipeline pressure; part of it is taken as feed for the ammonia plant and the rest is delivered as sales gas. Pure ethane, propane, butane and gasolines are plant products. Natural Gas Plant II has its cryogenic sector (referred to as Demethanizing Plant) several kilometres away from the conventional separation train (NGL Fractionation Plant). The demethanizing plant is fed with 36 MMm^3/d of natural gas. Light gases are separated from the heavy ones (ethane, propanes, butanes and gasoline) and injected to the natural gas pipeline. The feed mixture undergoes a conventional distillation train in the NGL Fractionation Plant to obtain LPG (Liquefied Petroleum Gas: propane, butane and gasoline) and ethane. Ethylene plants process 2,300 t/y of pure ethane; ethylene is provided as raw material to polyethylene and VCM plants and the rest is exported. The ammonia plant production is 2,050 t/d, most of which is fed to the urea plant to produce 3,250 t/d of urea. In these processes, 1.28 Mm^3/d of natural gas is used as raw material. Urea, ammonia, polyethylenes and PVC are delivered by ship, train and trucks.

3. Methodology

3.1. Life Cycle Optimisation of a Petrochemical Complex

The main objective of LCA is to provide quantitative environmental criteria in order to compare different alternatives of design and operational conditions. The first step of LCA is to set boundaries for the LCA analysis; defining the objective of the analysis, functional unit and environmental metrics, followed by identification and quantification of energy and material used within a process. The next step is the estimation of waste released to the environment. Obtained results are converted into a set of environmental impacts that can be aggregated into different groups, eighteen mid-point impact categories are proposed (Goedkoop et al., 2013). The ReCiPe 2008 impact assessment method has been used based on its better performance with respect to its predecessor method, Ecoindicator-99. LCA is integrated to optimisation tools to simultaneously evaluate the main operating conditions of a petrochemical complex. Environmental impact evaluation is performed following LCA principles, determined by ISO – 14040 (2015). The LCA is conducted in four steps: definition of goal and scope, life cycle inventory (LCI), life cycle impact assessment (LCIA) and interpretation.

Goal and Scope: The objective is to determine the petrochemical complex LCA. The functional unit of the LCA is the production in terms of tons of generated products.

Environmental impact is evaluated in transport, steam generation, emissions related to natural gas supply, electricity consumption and emissions of all operational units of the petrochemical complex. The impact is quantified by means of GWP metric and ReCiPe, which is the successor of Eco-Indicator 99 and CML-IA. The purpose is to integrate the 'problem oriented approach' of methodology CML-IA and the 'damage oriented approach' of methodology Eco-Indicator 99 (Goedkoop et al., 2013).

Life Cycle Inventory: This step aims to analyse all input/output data associated to the operation of the units of the petrochemical complex. The inventory of LCA is taken in transport, steam generation, emissions related to natural gas supply, electricity consumption and emissions of all operational units of the petrochemical complex.

Life Cycle Impact Assessment: Contributions corresponding to environmental impacts are calculated based on inventory analysis. GWP and ReCiPe are the metrics used to quantify environmental impact. Global Warming Potential (GWP) is calculated as the sum of GWP of each source of emission (Gebreslassie et al., 2013) and over a specific time horizon, Goedkoop et al. (2013) recommend a 100-year horizon. In ReCiPe, eighteen mid-point impact categories are proposed. These impact categories are aggregated into three damage models (damage to human health, damage to ecosystem quality and damage to resource) that are converted in only one ReCiPe measure. Damaging factors, which relate LCA results and impact categories, are given by the specific damage models available for each category (Goedkoop et al., 2013).

Interpretation: At this step, the calculated LCI and LCIA results are interpreted with respect to the goal and scope of the LCA study and recommendations for decision-making are given.

3.2. Mathematical Formulation

The life cycle optimisation of a petrochemical complex is formulated as an MINLP problem which determines the optimal operation of petrochemical complex considering the economic performance and environmental impact objective functions. Linear mathematical models have been derived for the NGL, ethylene and polyethylene plants, based on rigorous existing models tuned with actual plant data. Simplified models take into account variations in production with key plant operating variables, such as temperature and pressure in separation units. Available yield data for chemical transformations and utilities consumption have been used to model the rest of the petrochemical complex. Binary variables are associated to intermittent product delivery. MINLP models have been formulated with different objective functions: minimisation of GWP and multi-objective optimisation for profit maximisation and environmental impact minimisation, respectively. Approximate mixed integer linear models (MILP) have also been formulated applying linearization techniques to bilinear equations (Schulz et al., 2005) to obtain valid initial points for MINLP problems. The total profit is defined as the difference between sales revenue and total operating cost plus penalties for not meeting demands and inventory. Three major types of constraints are included in the model formulation: mass balance constraints, economic analysis constraints, and life cycle environmental impact constraints. A brief description of the plants and their mathematical models is given in Schulz et al. (2005). All model elements are calculated for the following components: CO_2, N_2, CH_4, C_2H_6, C_3H_8, C_4H_{10}, C_5H_{12}, C_6H_{14}, C_2H_4, C_3H_6, LDPE, LLDPE, HDPE, EPE, H_2, C_2H_2, C_4H_8, VCM, EDC, PVC, NH_3, $(NH_2)_2CO$.

Environmental constrains related to the optimisation problem are inventory analysis and environmental impact constraints. Inventory Analysis Constraints: Total emissions calculated in the LCI analysis (LCI_b^{tot}) consist of transport (LCI_b^{trans}), steam generation (LCI_b^{steam}), natural gas supply (LCI_b^{ng}), electricity consumption (LCI_b^{elec}) and operational unit (LCI_b^{emiss}) emissions of the petrochemical complex, as shown in Eq. (1):

$$\left(LCI_b^{tot}\right) = \left(LCI_b^{trans}\right) + \left(LCI_b^{steam}\right) + \left(LCI_b^{ng}\right) + \left(LCI_b^{elec}\right) + \left(LCI_b^{emiss}\right) \quad (1)$$

Different types of emissions are calculated according to emissions carbon footprint per functional unit and total consumption, as indicated in Eq. (2):

$$LCI_b^{cat} = LCIE_{b,cat}\bar{F}_{cat} \quad \forall\ b, cat\ \in \{trans, steam, ng, elec, emiss\} \quad (2)$$

where $\bar{F}_{cat}$ represents the total mass of transported raw material, total consumed cubic meters of steam water, total consumed cubic meters of natural gas, total kWh of electricity consumed, and total emissions released in kg during the operation of the petrochemical complex. LCI_b^{cat} corresponds to LCI input to the petrochemical complex of chemical species b in each unit.

Environmental Impact Constraints: Results from LCI are translated into different categories of environmental damage. GWP is calculated as the sum of GWP of each source of emission(GWP_{cat}), as indicated in Eq. (3).

$$GWP_{cat} = \sum_b LCI_b^{cat}\phi_{cat} \quad \forall cp, cat\ \in \{trans, steam, ng, elec, emiss\} \quad (3)$$

ϕ_{cat} is the damage factor that relates GWP of chemical species b to GWP. Damage factors of each type of greenhouse gases emissions are obtained from Solomon et al. (2007). Environmental performance is modelled minimising GWP.

$$GWP = \sum_b GWP_{cat} \quad (4)$$

ReCiPe: Environmental impact factors associated to each impact category are calculated from LCI analysis in Eq. (1) and damage factor of the model is calculated as follows:

$$IMP_c = \sum_b LCI_b d\, f_{bc} \quad \forall c \quad (5)$$

where IMP_c indicates the damage caused in the impact category c, LCI_b is the value associated to chemical species b in the LCI analysis and df_{bc} is the coefficient associated to chemical species b of the damage model c. These coefficients, that relate LCI analysis and impact categories, are given by specific damage model for each category and have been obtained with SimaPro (Ecoinvent Center, 2009). Finally, impact factors are aggregated into damage categories d (DAM_d), which are transformed into only one ReCiPe indicator, as follows:

$$DAM_d = \sum_{c \in CD(d)} IMP_c \quad \forall d \quad (6)$$

$$ReCiPe = \sum_d DAM_d nf_d w\, f_d \quad (7)$$

In Eq. (6), $CD(d)$ represents the different impact categories included in the damage category d. In Eq. (7), nf_d refers to factor normalisation and wf_d corresponds to factor weighing (Goedkoop et al., 2013). The MINLP bi-objective problem has been has been solved with the ε-constraint method (Guillén Gozalbez and Grossmann, 2009).

4. Numerical Results and Discussion

The MINLP model has 8,973 equations, 6,742 continuous variables and 200 binary variables. It is formulated in GAMS 24.1.3 modelling environment (Brooke et al., 2012) and solved with DICOPT (CONOPT3 and CPLEX). The MINLP problem is solved in eight major iterations. Each point of the Pareto optimal operations is generated in 2,503 CPU s. Optimisation results for GWP minimisation show that the petrochemical complex can satisfy product demands, while improving the environmental impact decreasing greenhouse emissions in almost 33 %, from 1,042 to 695.33 kt CO_2-eq/y in terms of GWP, while still fulfilling product demands and environment policies.

Figure 1 shows numerical results for the actual case study and after GWP minimisation, subject to all model constraints. They include GWP distributions associated to emissions, transport, steam usage, electricity and natural gas for the petrochemical complex. The main impact is given by associated emissions. Figure 2 shows environmental impact in terms of ReCiPe method and its eighteen mid-point impact categories after GWP minimization for the entire

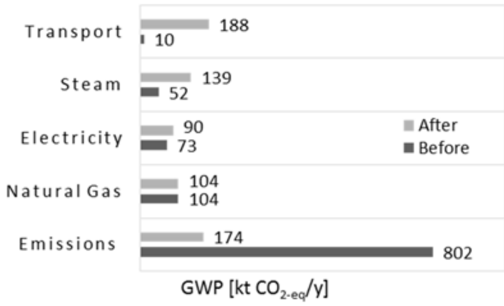

Figure 1: LCA for petrochemical complex (a) case study; (b) GWP minimisation

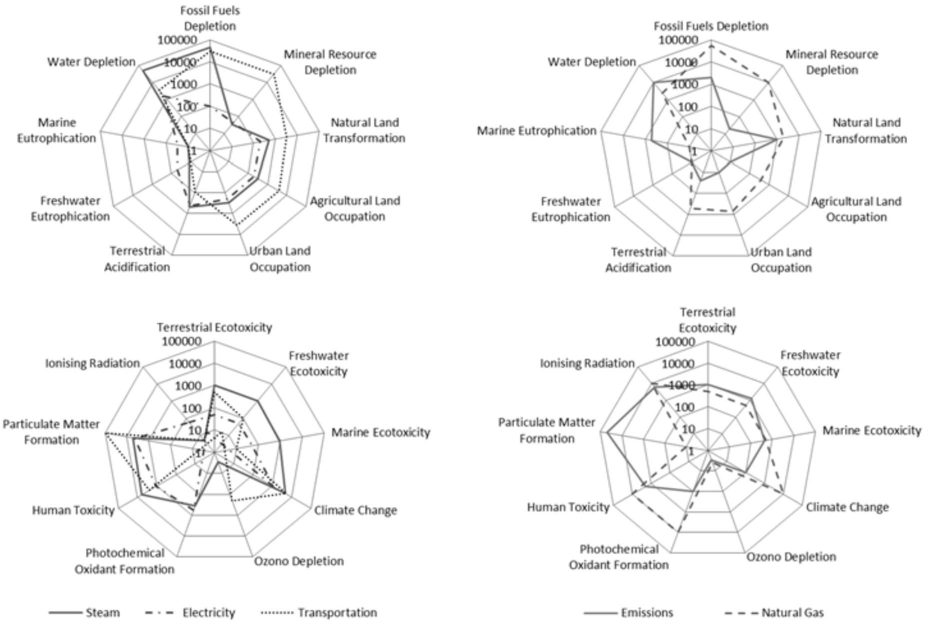

Figure 2: Mid-point Recipe impact factors in the entire petrochemical complex for steam, electricity. transport, emissions to the air and natural gas usage

petrochemical complex. The most important environmental impact is fossil fuel depletion, followed by mineral resource depletion, climate change and water depletion. The main impact is associated to process emissions, followed by natural gas usage, electricity, steam usage and transport. This is due to the fact that the main raw material is natural gas, which is transported by pipelines. Therefore, to reduce environmental impact, the main focus must aim at reducing emissions associated to each process unit. Figure 4 shows Pareto optimal solutions. GHG emissions can be reduced in 33 % with 24 % profit reduction, with respect to the case study (695.33 MMU$S and 1042.43 ktCO2eq/y, respectively), when minimising GWP. Optimal solutions also show that polyethylene plants have the best environmental performances in the entire complex.

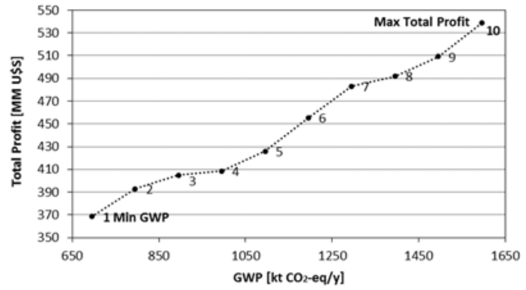

Figure 3: Pareto Curve for petrochemical complex

5. Conclusions

In this work, we formulate MINLP models for GWP minimisation and simultaneous optimisation of economic and environmental objectives for an operating petrochemical complex in Argentina. Including detailed process information within mathematical models provides deep insights into environmental behaviour. In our case study, optimisation results show that GRG emissions can be reduced in almost 33%, while still fulfilling product demands and environmental legislation.

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