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Highlights

Norberto García*, **Rubén Ruiz-Femenia**, **José A. Caballero**

EDUCATION FOR CHEMICAL ENGINEERS XXX (2012) XXX–XXX

Teaching mathematical modeling software for multiobjective optimization in chemical engineering courses

►Guidelines are introduced to incorporate environmental issues in a supply chain. ►It can be solved by undergraduate chemical engineering students. ►Computer programming skills are essential to solve real and complex systems. ►An algebraic modeling language facilitates to solve chemical engineering problems. ►The solution provides valuable insights into the design problem.

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Teaching mathematical modeling software for multiobjective optimization in chemical engineering courses

Q1 Norberto García*, Rubén Ruiz-Femenia, José A. Caballero

Department of Chemical Engineering, University of Alicante, Apto. de Correos 99, 03080 Alicante, Spain

ABSTRACT

This paper expects to give undergraduate students some guidelines about how to incorporate environmental considerations in a chemical supply chain and how the introduction of these concerns have an important effect on the results obtained in the multiobjective optimization problem where both economic and environmental aspects are considered simultaneously.

To extend the economic and environmental assessment outside the chemical plant and to identify the tradeoffs associated with the reality of chemical and petrochemical industries, a simplified problem of a chemical supply chain is proposed as a case study.

The inclusion of environmental concerns to this economic problem make this new case study a good example for undergraduate students interested in implementing simultaneous economic and environmental considerations in the chemical process design incorporating mathematical modeling software for solving this multiobjective problem.

Thus, the final objective of this paper is to show to undergraduate students how environmental together with economic considerations could have an important impact in the logistics of a supply chain and how multiobjective optimization could be used to make better decisions in the design of chemical processes including its supply chain.

To reach our purpose, the Pareto curve of the supply chain is obtained using the ε-constraint method. In addition, the tradeoffs of this multiobjective optimization have been identified and analyzed and ultimately a good decision based on the set of 'equivalent' optimal solutions for this chemical supply chain problem determined.

Keywords: Multiobjective optimization; Chemical process design; Post-secondary education; Economic and environmental assessment; The ε-constraint method

1. Introduction

Nowadays there is a growing awareness of developing students' computer skills in engineering courses. Computer-assisted learning is an essential tool to consolidate the theoretical concepts and to provide the future engineers with a strong competitive advantage for their careers. Thus, computer skills are core competencies for engineering graduates and it is expected that they will be taught to a greater extent (Law et al., 2010).

In the area of process systems engineering (PSE) the mathematical programming computer methods have led to successful results for real industrial applications (Grossmann, 2005; Guillén-Gosálbez et al., 2008; Gebreslassie et al., 2010; Kostin et al., 2010; Sabio et al., 2010). These optimization techniques are seldom taught to engineering students due to the modeling complexity of a real industry problem, which could lead with several hundred thousands of equations and variables. Moreover, the complexity of a real problem usually increases when the decision-maker desires to optimize simultaneously several performance indicators of the whole process. As a result the problem must be solved using a multiobjective optimization technique.

However, the solution of real process engineering optimization problems can be facilitated to the students by a powerful algebraic modeling language (such as GAMS, AMPL or AIMS), whose features allow students to formulate and solve these problems in reasonable time (Vannelli, 1993).

These modeling systems provide an algebraically based high-level language for the compact representation of large

* *Corresponding author.*
E-mail address: ngc2@alu.ua.es (N. García).

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Nomenclature

Indexes

i	manufacturing technologies
j	plants
k	warehouses
l	markets
c	raw materials

Parameters

$\overline{D_l^{MK}}$	maximum demand of product sold at market l [tons]
$\underline{D_l^{MK}}$	minimum demand of product to be satisfied at market [tons]
IMP_p^{RM}	cumulative LCIA results for the GWP associated with the consumption of one unit of raw material p [(kg $CO_{2\text{-eq}}$) (kg p)$^{-1}$]
IMP^{EN}	cumulative LCIA results for the GWP associated with the consumption of one unit of energy [(kg $CO_{2\text{-eq}}$) MJ^{-1}]
IMP^{TR}	cumulative LCIA results for the GWP associated with the transportation task of one unit of mass transported one unit of distance [(kg $CO_{2\text{-eq}}$) (tons km)$^{-1}$]
γ_l	price of the product sold at market l [\$ (tons)$^{-1}$]
γ_{jc}^{PU}	price of raw material p purchased at plant j [\$ ton^{-1}]
η_{ip}^{EN}	energy consumed per unit of chemical p produced with manufacturing technology i [TFOE (tons p)$^{-1}$], (Tons of Fuel Oil Equivalent = 41.868 GJ)
λ_{jk}^{PL}	distance between plant j and warehouse k [km]
λ_{jk}^{WH}	distance between warehouse k and market l [km]
μ_{ic}	mass balance coefficient associated with raw material p and manufacturing technology i [tons raw material c (tons product)$^{-1}$]
ψ_{jk}^{PL}	unitary transport cost of product sent from plant j to warehouse k [\$ (tons)$^{-1}$ km^{-1}]
ψ_{kl}^{WH}	unitary transport cost of product sent from warehouse k to market l [\$ (tons)$^{-1}$ km^{-1}]

Variables

C_{kt}^{WH}	capacity of warehouse k [tons]
W_{ij}	flow of product manufactured with technology i at plant j [tons]
W_{ijc}^{RM}	amount of raw material c consumed in technology i at plant j [tons]
PU_{jc}	purchases of raw material c made by plant j [tons]
Q_{jk}^{PL}	flow of product p sent from plant j to warehouse k [tons]
Q_{kl}^{WH}	flow of product p sent from warehouse k to market l [tons]
SA_l	sales of product p at market l [tons]

and complex models of varying types: linear (LP), nonlinear (NLP), mixed-integer linear (MILP) and mixed-integer nonlinear (MINLP). These problems, and specially the last one, appear often in chemical engineering process design and process integration. Algebraic modeling systems offer the students a compact way of writing complex models with thousands of equations and variables using index notation (Anwar and Bahaj, 2003; Kumar, 2001). The advantage of an algebraic modeling language is the similarity of their syntax to the common mathematical notation.

In education, optimization problems are sometimes solved by spreadsheet solvers (i.e., Excel) but it is not the common case for the real industry. Spreadsheet solvers are suitable for small problems, indeed it may be advantageous when the models are small enough; less than 30 equations and/or variables (Ferreira and Salcedo, 2001; Ferreira et al., 2004) but process engineers will have to cope with more complex systems along their careers. In teaching engineering, GAMS has been applied successfully by other authors (Mingo et al., 2011). These authors also take advantage of the feature of GAMS for combining easily with other widespread engineering software, MATLAB (Ferris, 1998) and improve student motivation towards learning certain topics in computer architecture (Anguita and Fernández-Baldomero, 2007).

Teaching GAMS in engineering courses is illustrated in this work through a simplified version of a case study taken from the supply chain management (SCM) discipline. SCM aims at the efficient integration of suppliers, manufacturers, warehouses and stores, in order to ensure that products are manufactured and distributed in the right quantities, to the right locations, and at the right time thereby maximizing the system's performance (Simchi-Levi et al., 2000). Under PSE approach, SCM involves the optimal integration of the operations of supply, manufacturing and distribution activities (Guillén-Gosálbez and Grossmann, 2010).

As we expect to teach undergraduate students the basis of multi-objective optimization, we propose a case study with two objectives: the economic, which is the traditional SCM performance indicator (Beamon, 1999), and the environmental performance. The choice of the latter criterion is motivated by the fact that, in the last decade, the trend of the incorporation of environmentally conscious decision-making in the SCM has gained wider interest (Guillén-Gosálbez and Grossmann, 2009; Grossmann and Guillén-Gosálbez, 2010). Furthermore, more and more technical universities now advocate integrating sustainability in higher education and including it as a strategic goal for improving education's quality and relevance to society (Ben-Zvi-Assaraf and Ayal, 2010).

Therefore, a large amount of research is currently being conducted for extending the scope of the analysis carried out in the PSE community in order to consider environmental aspects.

The aim of this work is to provide a modeling and computational framework to initiate engineering students in solving complex large-scale PSE multi-objective optimization problems. Specifically, we focus on the first stage of the learning curve, where the student becomes familiar with the GAMS modeling system language. After that stage, we show, from a practical perspective, how to implement a multi-objective solution procedure in GAMS.

The main contribution of our educational work is revealed when students have become practicing engineers, and thanks to the gained experience in our engineering courses, they are able to expand the modeling techniques into the real industrial context of process systems engineering and replace 'hand-on' experimentation which is complex and expensive (Magin and Reizes, 1990).

The paper is organized as follows. Section 2 presents a description of the proposed case study, including the problem statement and the mathematical formulation. In Section 3, the

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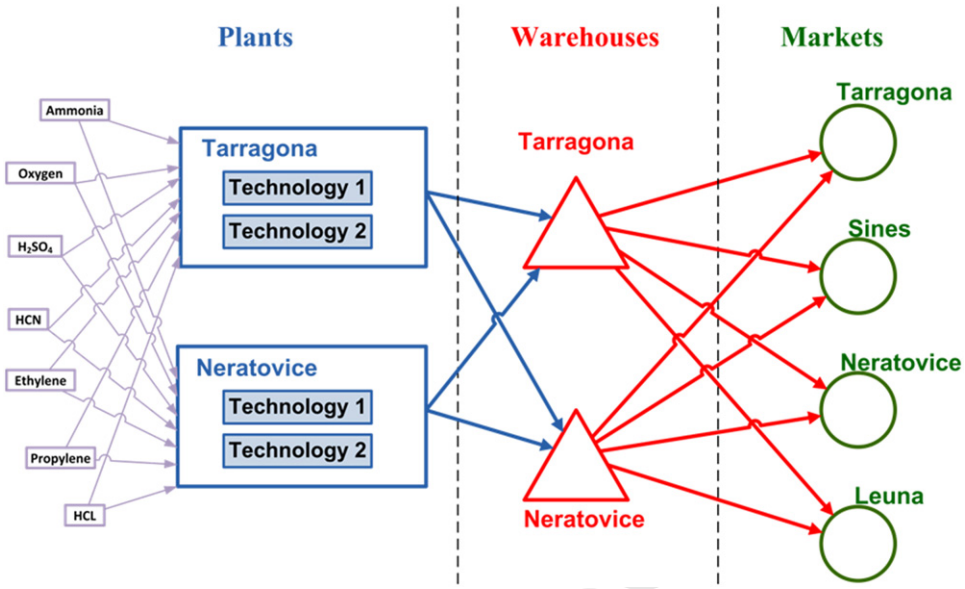

Fig. 1 – Superstructure of the supply chain problem.

multi-objective optimization method and its implementation in GAMS are presented. Section 4 describes the capabilities of the proposed modeling framework through the case study and the conclusions of the work are finally drawn is Section 5.

It is important to remark that in the University of Alicante, the students have a subject specific on applied optimization, besides the regular education in mathematics. In this course, there is an overview of mathematical programming theory (LP, NLP, MIP and MINLP) but the main focus is on correct modeling (i.e., avoid unnecessary non-convexities, models with binary variables, logical relationships, big-M and convex hull reformulations, etc.). In this context, it is also interesting introduce, the basic concepts on multiobjective optimization through 'small' examples related to actual problems.

2. Description of the case study

This supply chain (SC) problem addressed in this article is a simplified version based on that introduced by Guillén-Gosálbez and Grossmann for the optimal design and planning of real case of petrochemical supply chain (Guillén-Gosálbez and Grossmann, 2009).

The SC design problem proposed involves a petrochemical company which wants to set up in Europe to supply four important markets with a determined specific product through two plants and two warehouses situated in Tarragona (Spain) and Neratovice (The Czech Republic). The four markets are located in Tarragona, Sines (Portugal), Neratovice and Leuna (Germany).

With regards to the original problem statement introduced by Guillén-Gosálbez and Grossmann, we assume two major simplifications in order to make the original problem easily comprehensible to our students. The original problem is multiperiod, which implies different values for the variables in each of the time periods in which the total time horizon is divided. The problem aimed to our undergraduate students considers only one period of time and therefore all the variables are time-independent. The second simplification relies on the use of binary variables. The original mathematical formulation makes use of binary variables to take into account the planning of the expansion policy of the plants and warehouses during the total time horizon. We obviate the need for using binary variables due to our simplified problem is not multiperiod. Although it is out of the scope for an undergraduate course in PSE, once our students cope with the simplified version of the problem, it is not very complex to expand the mathematical formulation to include the multiperiod and expansion policy features. The former implies that the planning variables (production rates at the plants, flows of materials between plants, warehouses and markets and sales of products) depend on an additional set t which stands for the time periods. The inclusion in the model of binary variables implies the reformulation of some of the constraints with the convex hull representation for the disjunctions (Lee and Grossmann, 2000).

These two simplifications turn the original MILP (Mixed-Integer Lineal Programming) into a LP (Linear programming) problem.

Fig. 1 represents the superstructure associated with this supply chain problem.

Each plant can use two different manufacturing technologies to obtain the same product (acrylonitrile) using seven potential raw materials: ammonia, oxygen, sulfuric acid, hydrogen cyanide, ethylene, propylene and hydrochloric acid.

Fig. 2 represents the two potential technologies to obtain the acrylonitrile. It is also indicated in Fig. 2, the mass of raw materials consumed per unit of mass of acrylonitrile manufactured per each technology.

The capacity of each technology is limited to 3.5×10^4 tons of acrylonitrile and all raw materials have the same availability in each plant (4×10^4 tons).

The raw material costs are included in Table 1.

The variable costs associated with the two manufacturing technologies are indicated in Table 2. To avoid including binary variables and maintain the multiobjective model as simple as possible, fixed costs are not considered in this example.

The transport costs in each part of the supply chain could be calculated directly from the transport unit cost {0.01652 m.u./(ton km)} and the distances among the different markets that are shown in Table 3.

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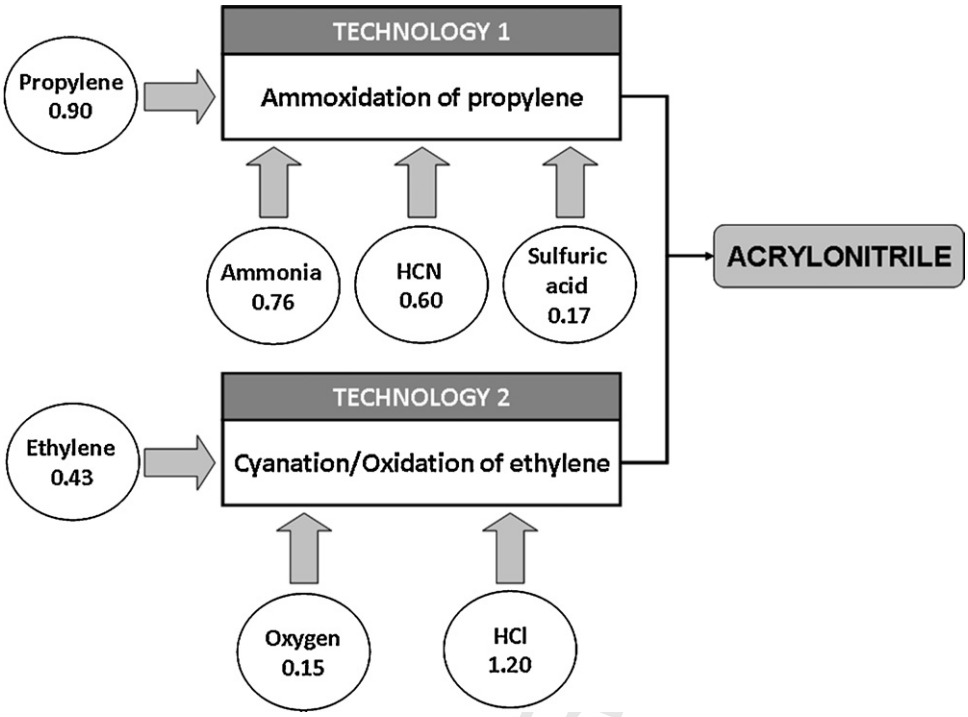

Fig. 2 – Description of the two manufacturing technologies with the mass of raw materials consumed per unit of mass of product (acrylonitrile).

Table 1 – Raw material costs at Neratovice and Tarragona plants.

Raw material	Costs of raw materials at plant (m.u.[a]/ton)	
	Neratovice	Tarragona
Ammonia	233.68	247.42
Oxygen	42.16	44.64
Sulfuric acid	116.18	123.02
HCN	468.47	496.03
Ethylene	140.54	148.81
Propylene	29.98	31.75
HCl	159.28	168.65

[a] m.u.: monetarian unit.

Table 2 – Variable costs associated with each potential manufacturing technology (m.u./ton).

Potential technology	Variable costs per plant (m.u./ton)	
	Neratovice	Tarragona
Technology 1	49.83	93.43
Technology 2	125.76	235.81

Furthermore, the company has to fulfill a minimum demand of product at each market. In addition, a company market research shows the maximum acrylonitrile demand and its most probable price at each market.

Table 4 shows the minimum and maximum demands of product at each market and their estimated prices.

For the environmental assessment of the supply chain (Guillén-Gosálbez et al., 2008; Guillén-Gosálbez and Grossmann, 2010; Ruiz-Femenia et al., 2011; Bojarski and Laínez, 2009), the Global Warming Potential (GWP) indicator has been used according to the Intergovernmental Panel on Climate Change (IPPC) (Hischier et al., 2010).

Table 5 shows the LCIA results associated with the raw materials manufacture, the energy consumption by utilities and the transportation tasks. All inputs are expressed as kg CO_2-equivalent/kg, kg CO_2-equivalent/MJ and kg CO_2-equivalent/(ton km), respectively. All the environmental impact values were retrieved from Ecoinvent Database (Frischknecht et al., 2004a,b,c).

The consumption of energy for each manufacturing technology, expressed as TFOE (Tons of Fuel Oil Equivalent), is included in Table 6.

So, the problem to be solved is to determine which manufacturing technology has to be used at each plant, which and how much raw materials have to be purchased, the production per plant and tons to be transported from each plant to the two warehouses (Tarragona and Neratovice) and tons to be sold at each market to maximize the benefits of the company (maximum profit) and minimize the environmental impact of the entire supply chain (minimum GWP).

3. Methodology

The supply chain problem has been modeled in GAMS (Brooke et al., 1998; McCarl, 2010; Mingo et al., 2011).

Table 3 – Distances between the plant locations and their markets.

PLANT	DISTANCES BETWEEN THE MARKETS AND THE PLANTS (km)			
	Leuna	Neratovice	Sines	Tarragona
Neratovice	259.84	0	2915	1924
Tarragona	1781	1924	1213	0

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Table 4 – Demands and prices of acrylonitrile at each market.

MARKETS	Minimum demand (tons)	Maximum demand (tons)	Prices of the product at each market (m.u./ton)
Leuna	7200	18,000	1092
Neratovice	20,000	50,000	1045
Sines	12,000	30,000	1053
Tarragona	6400	16,000	1072

Table 5 – Cumulative LCIA results for the Global Warming Potential (GWP) according to the Intergovernmental Panel on Climate Change (IPPC).

Environmental aspect	Raw material	Value	Units	DATASET Name from ecoinvent database
Raw materials consumption (IMP_p^{RM})	Ammonia (IMP_A^{RM})	2.9016	(kg CO_2-eq) kg^{-1}	Ammonia, partial oxidation, liquid, at plant
	Oxygen (IMP_B^{RM})	0.40915		Oxygen, liquid, at plant
	H_2SO_4 (IMP_C^{RM})	0.12406		Sulphuric acid, liquid, at plant
	HCN (IMP_D^{RM})	7.2893		Hydrogen cyanide, at plant
	Ethylene (IMP_E^{RM})	1.3989		Ethylene, average, at plant
	Propylene (IMP_F^{RM})	1.4379		Propylene, at plant
	HCl (IMP_G^{RM})	1.3123		Hydrochloric acid, from the reaction of hydrogen with chlorine, at plant
Energy consumption by utilities (IMP^{EN})	–	0.086141	(kg CO_2-eq) MJ^{-1}	Heavy fuel oil, burned in refinery furnace
Transportation tasks (IMP^{TR})	–	0.12105	(kg CO_2-eq) $(tons)^{-1}$ km^{-1}	Transport, lorry > 32 tons

Table 6 – Consumption of energy for each manufacturing technology.

Technology	η_{ip}^{EN} [FOET[a] $tons^{-1}$]
Technology 1	0.60
Technology 2	0.15

[a] FOET are the tons of Fuel Oil Equivalent and equivalent to 41.868 MJ.

The model equations are classified into three main blocks: mass balance equations, capacity constraints and objective function equations. These sets of equations together with the model variables are described next.

3.1. *Mathematical model*

A brief outline of each of these sets of equations, which have been implemented in GAMS, is next given.

In the equations given, the indexes refer to:

i: manufacturing technologies,
j: plants,
k: warehouses,
l: markets,
c: raw materials.

Furthermore, all abbreviations are also included at the end of the paper.

3.1.1. *Mass balance equations*

The mass balance must be satisfied for each node embedded in the network. Thus, for each plant j and raw material c, the purchases (PU_{jc}) must equal the total amount of raw material c consumed for each technology i at plant j (in tons):

$$PU_{jc} = \sum_i W_{ijc}^{RM} \quad \forall j, c \tag{1}$$

where PU_{jp} are the purchases of raw material p made by plant j (tons). W_{ijc}^{RM} is the amount of raw material c consumed in technology i at plant j (tons).Eq. (2) is added to represent the material balance for each technology i installed at plant j.

$$W_{ijc}^{RM} = \mu_{ic} W_{ij} \quad \forall i, j, c \tag{2}$$

In this equation, W_{ij} is the flow of product obtained with technology i at plant j (in tons), whereas μ_{ic} denotes the material balance coefficient for technology i and raw material c (in tons raw material c (tons product)$^{-1}$).

For each raw material, the purchases are constrained by an upper limit ($\overline{PU_{jc}}$), which are given by its availability in the current market place (in tons):

$$PU_{jc} \le \overline{PU_{jc}} \quad \forall j, c \tag{3}$$

For each plant j, the total amount of product transported between plant j and all the warehouses {Eq. (4)} must be equal to the total amount of product obtained for the two technologies installed at plant j (in tons):

$$\sum_i W_{ij} = \sum_k Q_{jk}^{PL} \quad \forall j \tag{4}$$

where W_{ij} is the flow of product manufactured with technology i at plant j (in tons) and Q_{jk}^{PL} is the flow of product transported from plant j to warehouse k (in tons).

Eq. (5) represents the mass balance for the warehouses. Here, the total amount of acrylonitrile transported from the

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two plants to the warehouse k must equal the material flow of product from the warehouse to all the markets:

$$\sum_j Q_{jk}^{PL} = \sum_l Q_{kl}^{WH} \quad \forall k \tag{5}$$

where Q_{kl}^{WH} is the flow of product sent from warehouse k to market l (in tons).

The sales of acrylonitrile at the markets (SA_l) are determined from the amount of materials sent by the warehouses, as it is stated in Eq. (6):

$$\sum_k Q_{kl}^{WH} = SA_l \quad \forall l \tag{6}$$

Eq. (7) forces the total sales of product at market l to be greater than the minimum demand target $\underline{D_l^{MK}}$ (in tons) and lower than the maximum demand ($\overline{D_l^{MK}}$) (in tons):

$$\underline{D_l^{MK}} \le SA_l \le \overline{D_l^{MK}} \quad \forall l \tag{7}$$

3.1.2. *Capacity and transportation constraints*

Eq. (8) constraints the production rate of technology i to be lower than a maximum production rate for each technology i ($\overline{W_i}$) (in tons):

$$W_{ij} \le \overline{W_i} \quad \forall i, j \tag{8}$$

The transportations flows between plants and warehouses (Q_{jk}^{PL}) and between warehouses and markets (Q_{kl}^{WH}) are constrained by upper limits (in tons):

$$\underline{Q_{jk}^{PL}} \le Q_{jk}^{PL} \le \overline{Q_{jk}^{PL}} \quad \forall j, k \tag{9}$$

$$\underline{Q_{kl}^{WH}} \le Q_{kl}^{WH} \le \overline{Q_{kl}^{WH}} \quad \forall k, l \tag{10}$$

3.1.3. *Economic objective function*

The economic performance of the supply chain is measured by the profit, which is given by the difference between the incomes (sales of products) and the total cost.

The revenues are determined from sales of the product ($):

$$\text{Sales of products} \equiv \sum_l \overbrace{\gamma_l}^{\$\cdot(\text{tons})^{-1}} \overbrace{SA_l}^{\text{tons}} \tag{11}$$

In this equation γ_l is the price of the product sold at market l ($ (tons)$^{-1}$).

The total cost includes the purchases of raw materials {Eq. (12)}, the operating costs associated with the two plants {Eq. (13)}, the cost of transporting materials between plants and warehouses {Eq. (14)} and between warehouses and markets {Eq. (15)}.

$$\text{cost of raw materials} \equiv \sum_j \sum_c \overbrace{\gamma_{jc}^{PU}}^{\$\,(\text{tons})^{-1}} \overbrace{PU_{jc}}^{\text{tons}} \tag{12}$$

$$\text{operating cost} = \sum_i \sum_j \overbrace{\alpha_{ij}}^{\$\,(\text{tons})^{-1}} \overbrace{W_{ij}}^{\text{tons}} \tag{13}$$

$$\text{transportation cost plant-warehouse} = \sum_j \sum_k \overbrace{\psi_{jk}^{PL}}^{\$\,(\text{tons})^{-1}\,\text{km}^{-1}} \overbrace{\lambda_{jk}^{PL}}^{\text{km}} \overbrace{Q_{jk}^{PL}}^{\text{tons}} \tag{14}$$

$$\text{transportation cost warehouse-market} = \sum_k \sum_l \overbrace{\psi_{kl}^{WH}}^{\$\,(\text{tons})^{-1}\,\text{km}^{-1}} \overbrace{\lambda_{kl}^{WH}}^{\text{km}} \overbrace{Q_{kl}^{WH}}^{\text{tons}} \tag{15}$$

In Eq. (12), γ_{jc}^{PU} denotes the prices of raw materials ($ ton^{-1}). In Eq. (13), α_{ij} is the production cost per unit of acrylonitrile manufactured with technology i at plant j.

Furthermore, ψ_{jk}^{PL} {Eq. (14)} and ψ_{kl}^{WH} {Eq. (15)} are the unit transport costs ($ (tons)$^{-1}$ km^{-1}).

Thus the economical objective function (in $) is:

$$\text{Profit} = [\text{Sales products } \{\text{Eq. (11)}\} - \text{Total costs}] \tag{16}$$

where:

$$\begin{aligned}\text{Total cost} &= \text{Cost of raw materials } \{\text{Eq. (12)}\} \\ &+ \text{Operating cost } \{\text{Eq. (13)}\} \\ &+ \text{Transportation cost plant-warehouse} \\ &\times \{\text{Eq. (14)}\} + \text{Transportation cost} \\ &\times \text{warehouse-market } \{\text{Eq. (15)}\}\end{aligned} \tag{17}$$

3.1.4. *Environmental objective function*

To assess the environmental performance of the supply chain, a combined approach that integrates Life Cycle Assessment principles with the optimization theory is followed (Azapagic and Clift, 1999a,b,c).

Life Cycle Assessment (LCA) is a quantitative environmental performance tool that applies the mass and energy balances to the complete system. In terms of the system boundary definition, this represents an extension to the conventional system analysis, in which the system boundary is drawn around the process of interest (Cano-Ruiz and McRae, 1998; Gutiérrez et al., 2010; Burgess and Brennan, 2001; Udo de Haes et al., 2002).

In this case study, the environmental impact of the supply chain is measured by the GWP indicator as it is described by the IPCC 2007.

Direct GWPs are relative to the impact of carbon dioxide in the atmosphere. GWPs are an index for estimating relative global warming contribution due to the atmospheric emission of a kg of a particular greenhouse gas compared to the emission of a kg of carbon dioxide. The unit of measurement is kg CO_2-eq or kilograms of carbon dioxide equivalent. A "*cradle-to-gate*" analysis to determine the total amount of global warming emissions released to the environment during the entire life of the supply chain is performed.

Three main sources of emissions that contribute to the GWP are considered: the consumption of raw materials (GWP^{RM}), the energy consumed by the utilities used in the

supply chain (GWP^{EN}) and the transportation of the materials between the nodes of the supply chain (GWP^{TR}). Hence, the total Global Warming Potential (GWP_{total}) is determined as follows:

$$GWP_{total} = GWP^{RM} + GWP^{EN} + GWP^{TR} \tag{18}$$

Mathematically, each source of global warming emissions could be expressed as a function of some continuous decision variables of the model. Specifically, they can be calculated from the purchases of raw materials (PU_{jp}), the production rates at the manufacturing plants (W_{ij}) and the transport flows (Q_{jk}^{PL} and Q_{kl}^{WH}) as stated in Eqs. (19), (20) and (21), respectively:

$$GWP^{RM} = \sum_{p} \overbrace{IMP_{p}^{EN}}^{(kgCO_2-Eq)\,(kg\,p)^{-1}} \sum_{j} \overbrace{1 \times 10^{3}}^{kg\,p\cdot(tons\,p)^{-1}} \overbrace{PU_{jp}}^{tons\,p} \tag{19}$$

$$GWP^{EN} = \overbrace{IMP^{EN}}^{(kg\ CO_2-Eq)\,MJ^{-1}} \sum_{i}\sum_{j} \overbrace{41 \times 10^{3}}^{MJ\,(TFOE)^{-1}} \overbrace{\eta_{ip}^{EN}}^{TFOE\cdot(tons)^{-1}} \overbrace{W_{ij}}^{tons} \tag{20}$$

$$GWP^{TR} = \overbrace{IMP^{TR}}^{(kg\ CO_2-Eq)\,(tons\,km)^{-1}} \left(\sum_{j}\sum_{k} \overbrace{\lambda_{jk}^{PL}}^{km} \overbrace{Q_{jk}^{PL}}^{tons} + \sum_{k}\sum_{l} \overbrace{\lambda_{kl}^{WH}}^{km} \overbrace{Q_{kl}^{WH}}^{tons} \right) \tag{21}$$

In Eqs. (19)–(21), IMP_{p}^{RM}, IMP^{EN} and IMP^{TR} denotes the cumulative LCIA results for the GWP associated with the consumption of 1 kg of raw material p, 1 MJ of energy and the transportation of 1 ton 1 km, respectively (their values have been directly downloaded from the Ecoinvent database and they are shown in Table 5).

In Eq. (20), η_{ip}^{EN} represents the consumption of energy per unit of product manufactured with technology i (their values are indicated in Table 6). It includes utilities such as electricity, steam, fuel and cooling water, which are converted into Tons of Fuel Oil Equivalent (TFOE) where 1 TFOE is equivalent to 41.868 GJ.

Thus, the life cycle impact assessment of the generation and supply of thermal energy from the combustion of one unit of fuel oil can be used to estimate the consumption of utilities.

In Eq. (21), λ_{jk}^{PL} and λ_{kl}^{WH} denote the distance between the plants and the warehouses and from the warehouses to the markets, respectively (in km).

3.2. *Solution procedure for the multiobjective optimization*

The main purpose of this example is to the introduce concept of multiobjective optimization to undergraduate students. Consequently, the supply chain should be designed and optimized according to both criteria: economic and environmental performance.

Hence, students have to deal with a multiobjective problem that could be formulated as follows:

$$(M) \quad \begin{array}{l} \max_{x} \{Profit(x); -GWP_{total}(x)\} \\ s.t. \quad Eqs.\ (1)–(21) \end{array} \tag{22}$$

Here, x generically denotes the continuous variables. Note that as the improvements in economic and environmental objectives are in opposite directions, maximizing Profit and minimizing GWP, respectively, we add the negative sign to the GWP to set the same search direction for both objectives. This formulation is equivalent to maximize Profit and minimize GWP and eases its implementation in GAMS.

The SC design with higher profit will lead to higher values of the environmental impact, so they tend to be contradictory objectives. Thus, the solution of the multiobjective problem is not unique but rather a set of alternative optimal designs (i.e., Pareto-optimal points) representing the trade-off among the two objectives. The set of Pareto-optimal points (or Pareto curve) contains the non-inferior solutions, which are the ones in which an improvement in one of the objective requires a degradation of another.

In this work, the Pareto solutions are determined via the ε-constraint method (Ehrgott, 2005; Mavrotas, 2011) which entails solving a set of instances of the following single-objective problem M1 for different values of the auxiliary parameter ε:

$$(M1) \quad \begin{array}{l} \max_{x} \{Profit\} \\ s.t. \quad Eqs.\ (1)–(21) \\ GWP_{total} \le \varepsilon \\ \underline{\varepsilon} \le \varepsilon \le \bar{\varepsilon} \end{array} \tag{23}$$

where the lower ($\underline{\varepsilon}$) and upper ($\bar{\varepsilon}$) limits within which the epsilon parameter must fall are obtained from the optimization separately of each objective:

$$(M1a) \quad \begin{array}{l} (\bar{x}) = \underset{x}{\operatorname{argmax}}\{Profit\} \\ s.t. \quad Eqs.\ (1)–(21) \end{array} \tag{24}$$

which defines $\bar{\varepsilon} = GWP\,(\bar{x})$ and

$$(M1b) \quad \begin{array}{l} \underline{GWP_{total}} = \min_{x}\{GWP\} \\ s.t. \quad Eqs.\ (1)(21) \end{array} \tag{25}$$

which defines $\underline{\varepsilon} = \underline{GWP_{total}}$.

4. Model implementation in GAMS

The main motivation for using GAMS lies in its ability to write down indexed equation blocks in a very compact form that will generate automatically a large amount of single equations.

As an example, Fig. 3 shows the transformation of the environmental equations of the proposed supply chain model from mathematical notation into the GAMS language. It is remarkable that there is a high similarity between mathematical and GAMS notation.

A crucial algebraic modeling element is the identification of indices (also referred to mathematically as a subscript).

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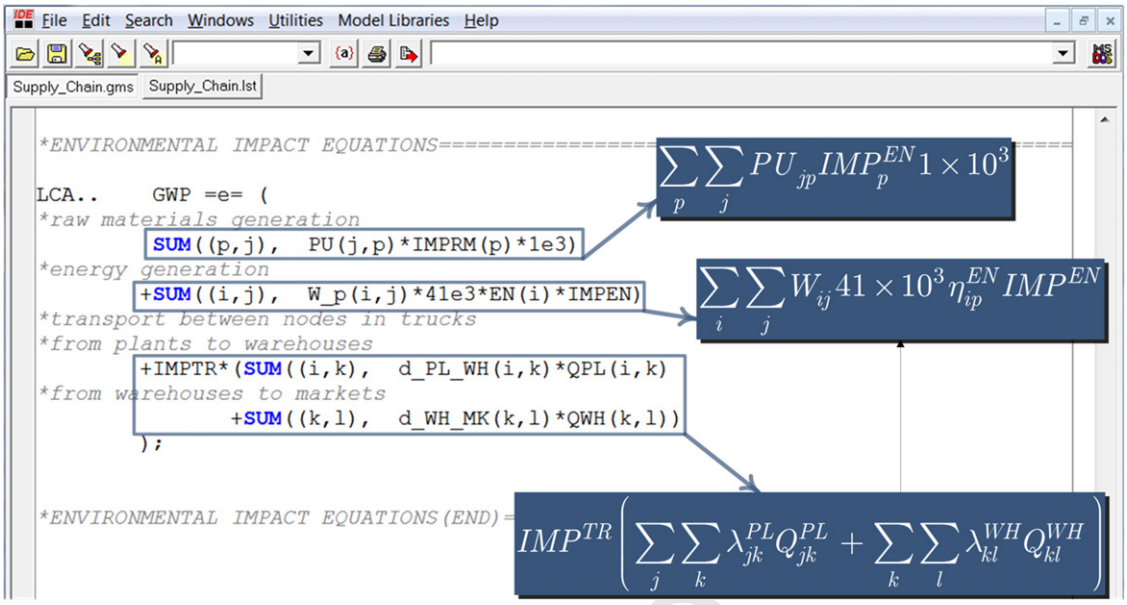

Fig. 3 – Screenshot of the environmental equations implemented in GAMS. It is also shown the same equations in mathematical notation.

Definition of indices in GAMS involves the definition of sets and set elements. Namely, an index in mathematical summation notation is a set in GAMS and the summation over the subscripts p and j in Eq. (19) is specified in GAMS by the summation operator "SUM", followed by the name of the sets separated by a comma within parentheses "(p, j)" (Fig. 3) (Salcedo-Díaz et al., 2011; Haimes et al., 1979).

Note that the structure for specifying a constraint equation in GAMS requires the specification of an equation name (for the equation in Fig. 3 we use "LCA") followed by two periods and then the algebraic statement. At the end of the expression, a semicolon must be typed. The indication of the form of the inequality appears as "=L=" for less than or equal to; "=G=" for greater than or equal to and "=E=" for equal to.

The implementation of the ε-constraint method in GAMS is illustrated in Fig. 4.

The first step is the calculation of the lower ($\underline{\varepsilon}$) limit. In the GAMS program we start by solving the single-objective M1b problem {Eq. (25)}. This task is accomplished by invoking the solver with the reserved word "SOLVE" followed by the name of the model ("SCM_LCA"), then it comes after, the reserved word "using", the direction of the optimization ("minimizing") comes next and finally the objective function variable name ("GWP"). Once the first single optimization problem is solved, the minimum value of the objective function variable "GWP.l" is stored in the parameter "GWP_lo", which corresponds to the lower limit ($\underline{\varepsilon}$).

Similarly, as with the lower limit, we calculate the upper ($\bar{\varepsilon}$) limit, but for this case, the objective function variable maximized is "profit", and the results are assigned to the parameter "GWP_up". Next stage fulfills the solving problem (M1) for each Pareto point. This requires the definition of a set with the number of Pareto points, "p", and a counter variable "ITER". Here we use the "loop" statement controlled by the set "p" to solve repeatedly the problem (M1). For each Pareto point we store the optimize values of the Profit and the GWP in the parameters "Profit_p" and "GWP_p", respectively. The last line inside the loop performs the updating of the epsilon parameter.

Once the ε-constraint method is applied, it is possible to obtain the Pareto curve (Fig. 5).

If the Pareto curve is analyzed, there is a clear trade-off between the economical indicator (Profit) and the environmental indicator (GWP_{total}), since reductions in the environmental impact (GWP_{total} reductions) can only be achieved by compromising the economic performance which involves reducing profits (Gebreslassie et al., 2009).

There is also indicated in Fig. 5 the extreme solutions of the Pareto curve (or p-anchor points) which are those that correspond to the minimum environmental impact (minimum GWP_{total}) and the maximum economic performance (maximum profit) for this multiobjective problem.

In addition to these extreme points, there are 18 points that represent intermediate solutions (non-inferior Pareto solutions) which are also local optimums.

4.1. *Minimum GWP_{total} (environmental optimum)*

Fig. 6 shows the supply chain configuration for the extreme solution corresponding to the minimum environmental impact (minimum Global Warming Potential, GWP_{total}) or the environmental optimum.

Inside the blue boxes are the capacities of each technology (in tons per year). For each plant is also shown the production of product manufactured. Red boxes represent the two warehouses and green boxes the four markets. The blue and green arrows represent the flow of materials between the plants and the warehouses and between the warehouses and the markets, respectively.

This extreme solution (minimum GWP_{total}) entails the production in both plants (Tarragona and Neratovice) using only the second technology because it has the lowest environmental impacts.

In this scenario, the number of transportation links between the warehouses and the markets are kept very low and the markets are only provided by the closest warehouses. It means that, in the minimum GWP_{total} solution, the product is manufactured as close as possible to the final markets. It implies that this supply chain topology tries to reduce the carbon dioxide emissions due to the transportation tasks.

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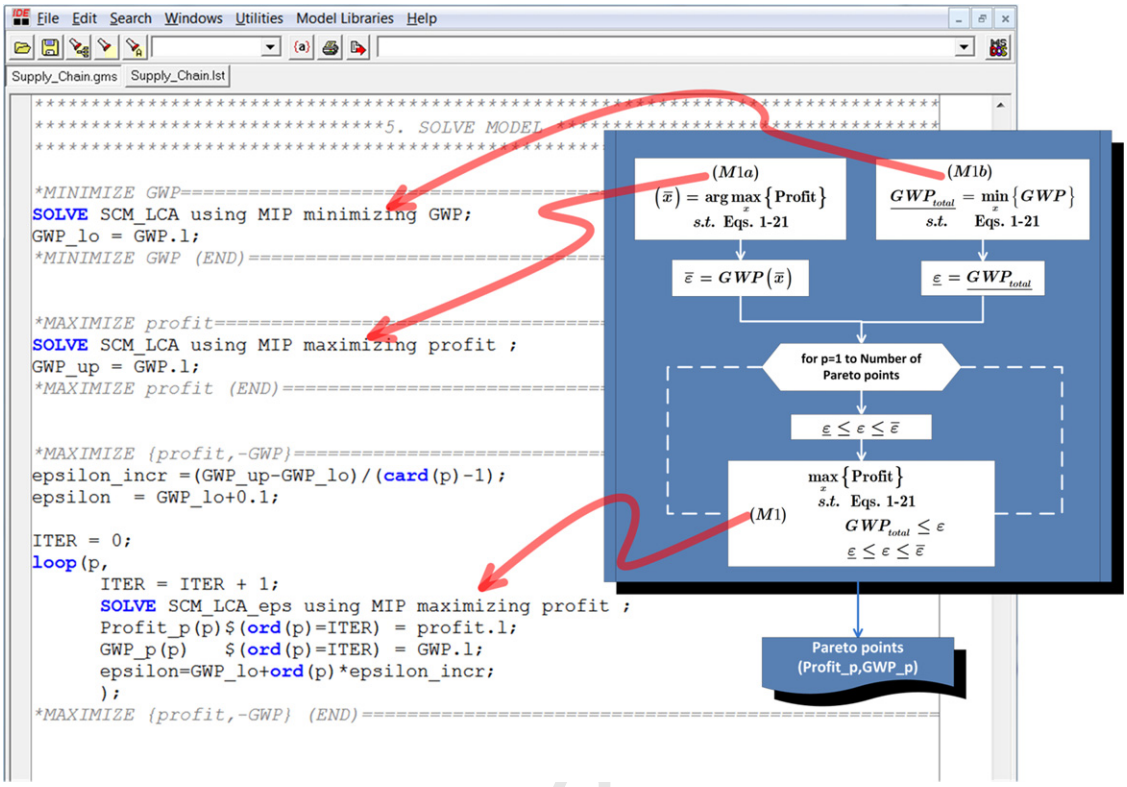

Fig. 4 – Implementation of the ε-constraint method in GAMS.

Another point to be remarked lies in the SC capacity, which is lower in the minimum environmental impact design.

In this environmental solution, the production rates are reduced and the demand satisfaction level drops to its lower limit. The lower product to be manufactured and transported, the lower impact the supply chain has.

4.2. *Maximum profit (economic optimum)*

Fig. 7 describes the supply chain configuration of the extreme solution corresponding to the maximum profit solution (or economic optimum).

This solution entails both plants (Tarragona and Neratovice) but, using both technologies (1 and 2) in order to reach high production capacities.

In this scenario (maximum profit), the number of transportation links between the warehouses and the markets are kept very high and the markets are provided by all warehouses. There are some exceptions: Tarragona market is only provided by the Tarragona warehouse and Leuna by the Neratovice one.

In the maximum profit solution, part of the total production is made in the plant of Neratovice and then shipped to the warehouse that is close to the existing plant located in

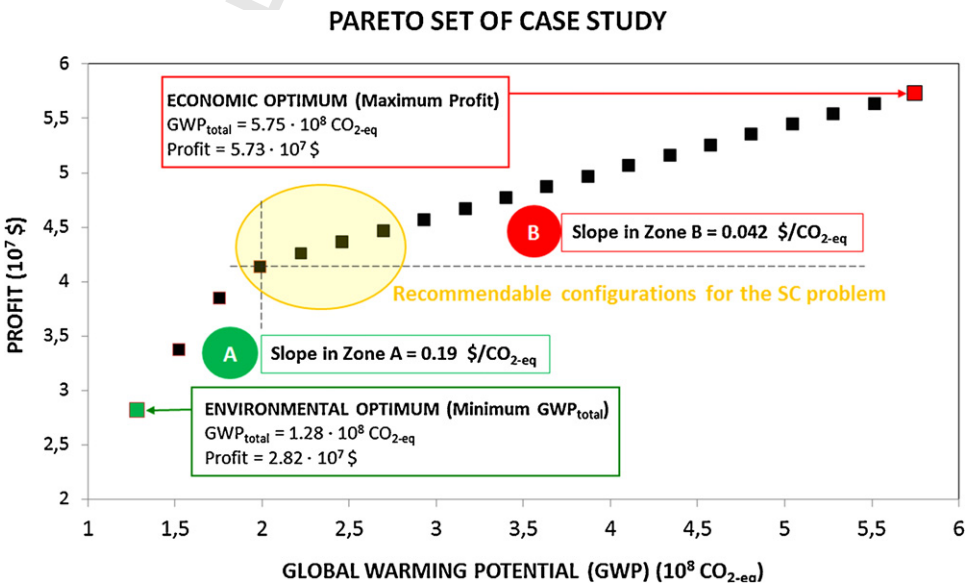

Fig. 5 – Pareto solutions set of the supply chain problem.

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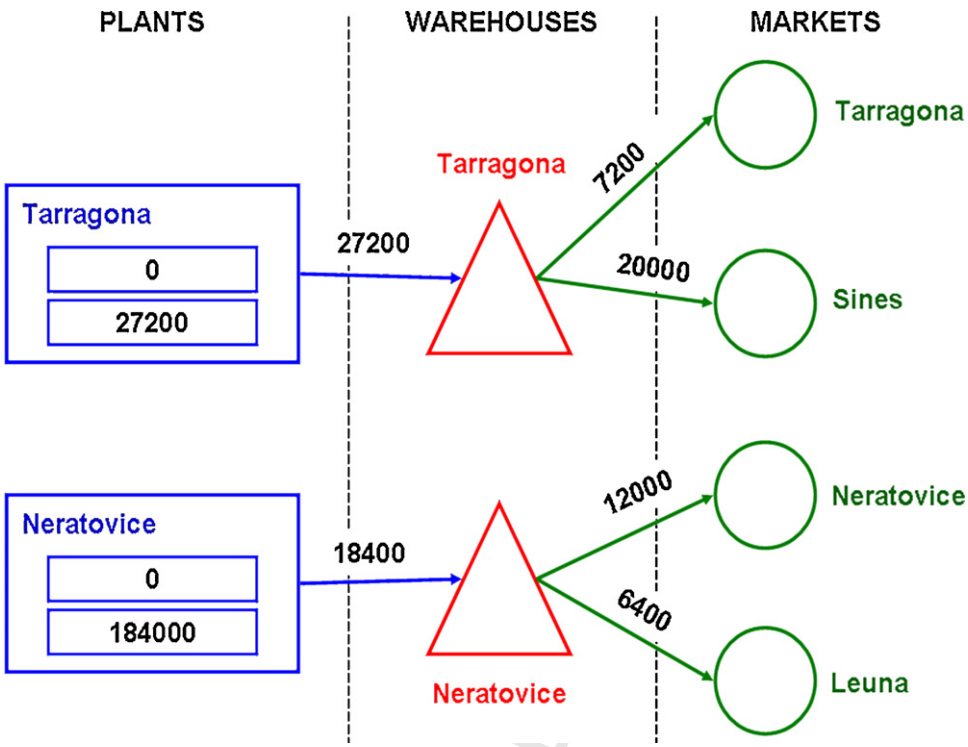

Fig. 6 – Minimum GWPtotal solution (Environmental Optimum).

Tarragona. By doing so, the model takes advantage of the lower production costs in the Czech Republic compared with Spain.

In addition, there are 18 intermediate non-inferior solutions that are also acceptable. It will be the process engineer who should determine attending to his/her criteria what it is the best configuration for this SC problem.

Thus, in the zone A (Fig. 5) there is an increase of profit without increasing a lot the environmental impact of the supply chain. However, in the zone B (Fig. 5), the increase of profits involves a high increment of the environmental impact. It becomes evident if we compare the slopes of the lines in the zone A (0.19 \$/$CO_{2\text{-eq}}$) with the slope of the line in zone B (0.042 \$/$CO_{2\text{-eq}}$).

So, if we attend to environmental concerns, we should move on the left of the zone A to reach "good" environmental performances (less environmental impacts than in zone B) and "acceptable" profits (less profits than in zone B).

If we only want to minimize the environmental impact, the best solution would be the environmental optimum ($GWP_{total} = 1.28 \times 10^8$ $CO_{2\text{-eq}}$; Profit $= 2.82 \times 10^7$ \$). However, if

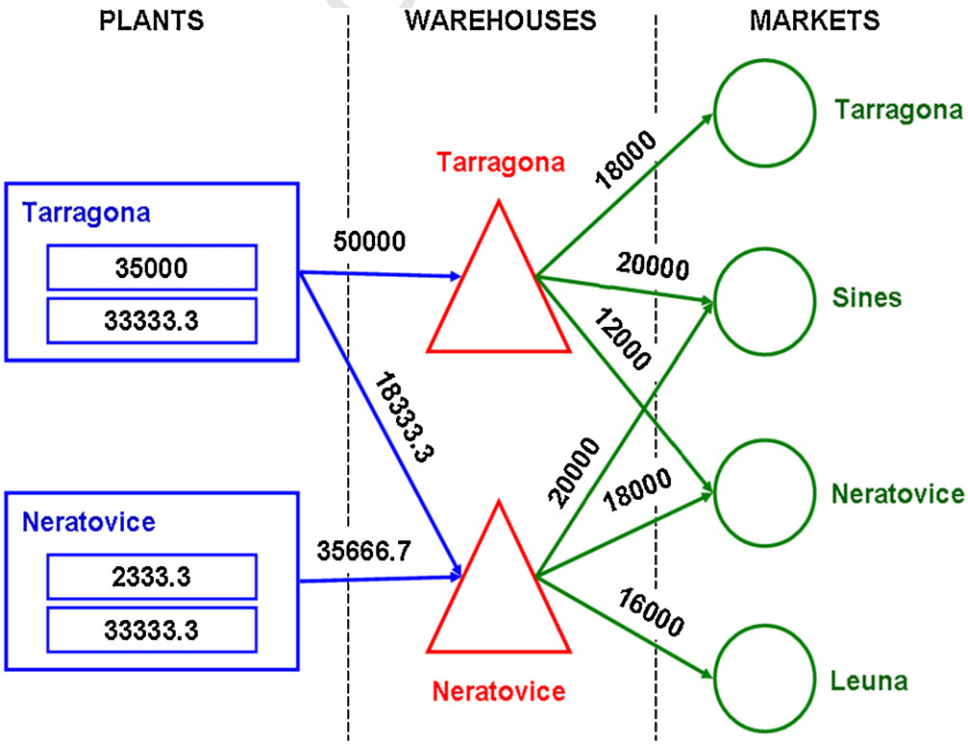

Fig. 7 – Maximum profit solution (Economic Optimum).

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we are interested in economic issues, we should move at the beginning of the zone B to obtain "good" profits (higher than in zone A) and "acceptable" environmental impacts (higher than in zone A). Attending only to the economic criterion, the best solution would be the economic optimum ($GWP_{total} = 5.75 \times 10^8\ CO_{2\text{-eq}}$; Profit = 5.73×10^7 \$)

So, attending to both criteria, the recommendable area is situated between zone A and B (Fig. 5). In this area (indicated as a red circle in Fig. 5) allows reaching "acceptable" profits and environmental impacts. These points are good solutions of the system because they allow to obtain more than the 70% of the maximum profit (between 4 and 4.5×10^7 \$) increasing only 70% the minimum environmental impact (between 2 and $2.75 \times 10^8\ CO_{2\text{-eq}}$).

5. Conclusions

This paper wants to emphasize undergraduate students how real environmental indicators (i.e., Global Warming Potential) could be used simultaneously with optimization tools (Pareto analysis and the ε-constraint method) to determine the best solutions to a typical supply chain problem.

Furthermore, the facility to implement this problem in GAMS let introduce the basis of multiobjective optimization and how identify the best tradeoffs for this type of problems.

Thus, students who are worried about environmental concerns (or attending to environmental laws or regulations) would work with supply chain configurations near the environmental optimum (GWP_{total}) or vice versa if they are interested in the economic terms.

The analysis of the Pareto curve allows to identify two zones with different ratios of profit increase to GWP increase (slope). The first part of the curve (zone A) has the highest value of the slope (0.19 \$/$CO_{2\text{-eq}}$) and comprises the SC designs that provide the lowest values for both indicators (environmental concern solutions, zone A of Fig. 5). The second part (zone B) with the lowest value of the slope (0.042 \$/$CO_{2\text{-eq}}$) corresponds to the SC configurations giving the highest values for the two indicators (profit-taker, Zone B of Fig. 5). In zone A, the decision-maker can choose a design with a higher profit leading only to a small increment in the GWP. Whereas the lower value of the slope in zone B prompts the decision-maker to adopt a conservative increase of the profit in order not to exceed the GWP level.

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