Sustainability Analysis of Industrial Processes

Henrique A. Matos and Ana Carvalho

Abstract Our planet has been extensively impacted by the enormous consumption of natural resources and due to the high level of emissions coming from the productive systems. This situation is imposing severe burdens to the planet, leading to environmental disturbances and a huge level of pollution, which is causing a significant increase of human diseases. Sustainability Analysis at the industrial process level is mandatory to accomplish the sustainable development among nations. The aim of this chapter is to clearly present the sustainability agenda across the past decades and integrate that concept in the industrial processes analysis. For that, metrics and tools available to assess and improve industrial processes in terms of sustainability are presented. Some examples of the application of these tools are also described.

Keywords Sustainability · Process design · Indicators · Sustainability tools

1 Introduction

Resources are becoming scarce and the planet will not last long with the current levels of consumption, of fossil fuels, minerals, among other resources. The industrial productive system is responsible for the production of products and services, required to meet the demanding standards of a consumerist population. The major problem in this civilization is the use amount of resources extract from the nature, and out of that only 20 % in terms of weight is effectively used (OECD 2012). The remaining resources are wasted in different ways, gaseous emissions, liquid effluents and solid disposals. Due to the aforementioned situation, a strong

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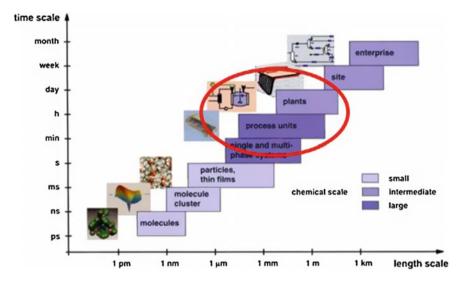


Fig. 1 Multi-scale approach in process systems engineering (WRI 2005)

activity has been carried out in the industrial production sites in order to improve the sustainability of the industrial processes. Among the scientific/technical developments it can be highlighted the new and more efficient catalysts and more efficient separations through the integration of new agents. Moreover, the industrial process intensification and integration attitudes, also move the processes towards the right direction, leading to systems, which seem to have all the plant inside of an environment-friendly container, sometimes called the "Banana Container".

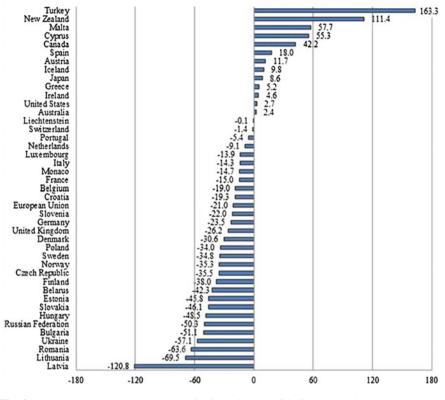
In order to obtain a more efficient and environmental friendly productive industry, a holistic vision, covering a complete multi-scale approach is required. The multi-scale approach spans from the molecule level through all supply chain management, considering sustainable suppliers and final adequate disposal of the non-used items (Fig. 1).

This chapter will be dedicated to a cornerstone of any supply chain, the production process. This chapter aims to present the concept of sustainability and how they should be integrated in the Sustainability Analysis of Industrial Processes. For that purpose the methodologies and indicators suitable for sustainability improvement and assessment at the process level, will be revised. This chapter is organized as follows. In the next section an overview of the sustainability concept will be presented. In Sect. 3 the assessment methodologies for the three pillars of sustainability are described. Then in Sect. 4 the integrated methodologies for process improvement towards sustainability are presented. Conclusions are presented in Sect. 5.

2 Sustainability Analysis Concept

The widespread awakening on the issue of sustainability in the development of society was made during the decade of the 60s of the twentieth century. However, sustainability has only been considered a landmark, achieving the public recognition, with the publication of the book Limits to Grow in 1972 by Meadows et al. (1972). This book was the result of a group of industrialists who gathered in Rome to discuss the "new" international problems. This work describes the results of a computer model of human evolution ("World 3"), which identifies the consequences for the planet, of the current exponential industrial development and population growth. The book's conclusions are something catastrophic, and are based on scenarios away from the reality of a finite world. These conclusions had a strong impact on public opinion and especially in political power.

Later, in 1992, the same research group published an updated work through the book Beyond the Limits (Meadows et al. 1992), and the findings were similar to the previous edition, which showed that much work was still required. The concept of Sustainability was formally introduced by the World Commission on Environment and Development (WCED) of the UN headed by the Prime Minister of Norway, Gro Harlem Brundtland in the report "Our Common Future" or Brundtland Report (Brundtland 1987). In this report sustainability has been defined as: "meet the needs of the present generation without affecting the ability of future generations get their supply." The report indicates a number of measures that should be taken by countries to promote sustainable development. One of the proposed measures, in the Brundtland report, concerns the need for the United Nations (UN) to implement a sustainable development program. This recommendation of the commission led to the development of Agenda 21 that began in 1989 with the approval of a special meeting with the United Nations, in a conference on environment and development. All member states of the UN developed a complex process of review, consultation and negotiation, culminating in the Second United Nations Conference on Environment and Development, known as Rio-92 or Eco 92, held in Brazil. There, representatives of 179 governments agreed to adopt a deep programme on the subject Agenda 21 had a close monitoring from which were made adjustments and revisions. The first step was the Rio+5 conference in 1997, at UN Headquarters in New York; later with the adoption of an additional calendar called the Millennium Development Goals (Millennium Development Goals), with particular emphasis on globalization policies and the eradication of poverty and hunger, adopted by 199 countries at the 55th UN General Assembly, held in 2000 at New York; The Declaration of the Millennium Development Goals outlined eight basic objectives, which are (Almeida, 2007): (1) Eradicate extreme poverty and hunger; (2) Achieve universal primary education; (3) Promote gender equality and empower women; (4) Reduce child mortality; (5) Improve maternal health; (6) Combat HIV, malaria and other diseases; (7) Ensure environmental sustainability; (8) Develop a global partnership for development.



Changes in GHG emissions including LULUCF (%)

Fig. 2 Total aggregate greenhouse gas (GHG) emissions of individual parties including Land Use, Land-Use Change and Forestry (LULUCF), 1990–2012 (UNFCCC 2015)

Meanwhile, the Kyoto Protocol is an international agreement linked to the United Nations Framework Convention on Climate Change, which commits its Parties by setting international binding emission reduction targets. Recognizing that developed countries are principally responsible for the current high levels of GHG emissions in the atmosphere as a result of more than 150 years of industrial activity. During the first commitment period, 37 industrialized countries and the European Community committed to reduce GHG emissions to an average of 5 % against 1990 levels. During the second commitment period, Parties committed to reduce GHG emissions by at least 18 % below 1990 levels in the eight-year period from 2013 to 2020; however, the composition of Parties in the second commitment period is different from the first as shown in Fig. 2 where the GHG are accounting including Land Use, Land-Use Change and Forestry (LULUCF).

Some other Summits on Climate Changes and Sustainable Development were carried out such as the Summit in Johannesburg, South African in September 2002,

Copenhagen in 2009, Cancun in 2010 and Rio+20 in 2012. All occur to establish more targets and assess the countries performance.

In 25–27 of September, 2015 the United Nations Development Summit defined the new Agenda 2030, which is a plan of action for people, planet and prosperity. It also seeks to strengthen universal peace in larger freedom. Eradicating poverty in all its forms and dimensions, including extreme poverty, is the greatest global challenge and an indispensable requirement for sustainable development. All countries and all stakeholders, acting in collaborative partnership, will implement this plan. The new 17 Sustainable Development Goals (SDG's) and 169 targets, which are announced at that summit demonstrated the scale and ambition of this new universal Agenda. The SDG's and targets will stimulate action over the next fifteen years in areas of critical importance for humanity and the planet:

- People To eradicate the poverty and hunger, in all their forms and dimensions, and to ensure that all human beings can fulfil their potential in dignity and equality and in a healthy environment.
- Planet To protect the planet from degradation, including sustainable consumption and production, sustainable managing its natural resources and taking urgent actions on climate change, so that it can support the needs of the present and future generations.
- Prosperity To ensure that all human beings can enjoy prosperous and fulfilling lives and that economic, social and technological progress occurs in harmony with nature.
- Peace To foster peaceful, just and inclusive societies, which are free from fear and violence. There can be no sustainable development without peace and no peace without sustainable development.
- Partnership To mobilize the means required to implement this Agenda through a revitalised Global Partnership for Sustainable Development, based on a spirit of strengthened global solidarity, focussed in particular on the needs of the poorest and most vulnerable and with the participation of all countries, all stakeholders and all people.

The concept of sustainable development must be assimilated by the leaders of the companies as a new way to produce without degrading the environment, extending this culture at all levels of the organization. A systematic analysis of the company's production process in terms of impact on the environment, economic and social aspects should be conducted. This analysis should result in the implementation of a project, which combines production, social and environmental preservation, with technology adapted to that principle (Ramôa Ribeiro 2009). Sustainability Analysis of Industrial Processes emerges as an indispensable practice to design and evaluate new processes and/or existing ones (retrofit design). It is essential to assess the existing process and propose new design alternatives in terms of the three pillars of sustainability. The three main components of sustainability analysis in industrial processes are accordingly to its basic definition the following:

- Stability and cost-effectiveness: should be sought technological solutions that lead to optimum operating point at the level of minimum total cost or maximum profitability;
- Ecological balance: by including the rational use of raw materials, the preservation of natural ecosystems and mitigating the effects of climate change;
- Social development and equity: adapting the existing rule to the concrete situation, observing the criteria of safety, justice and equality.

3 The Sustainability Pillars and Their Assessment

Sustainability is comparable to a tripod where each leg corresponds to a specific pillar: Economic, Environmental and Social. It makes no sense to walk in each of the fields independently, but instead these fields should be harmonized in order to achieve an appropriate outcome. To attain this goal, it is required to have methodologies and tools, which deal with the three pillars of sustainability. It is also required to incorporate sustainability indicators, covering the different areas, so that industrial processes can be assessed.

3.1 Methodologies and Tools to Address the Economic Pillar

Several approaches could be used to successful employ the sustainability economic pillar, however in the industrial process studies the best practice is through process modelling and optimization. The descriptive mathematical models of the processes, through equality or inequality constraints is added to an economic objective function usually based on operating costs or profit. A possible technical-economic solution should be found, corresponding to the best value for a given objective. This means the optimal operational conditions are set to the variables, leading to the minimum cost or maximum profit.

Several commercial software packages with a modular structure or individual components are used to solve the representative model resolution sequentially (e.g. ASPEN Plus, PRO-II or HYSYS). Some illustrative of the Aspen Suite interface and results are shown in Fig. 3.

Alternatively, a simultaneous resolution of the mathematical model could be chosen. Some models equation-based written in language as *gPROMS* (http://www.psenterprise.com/company.html) can be used to describe process steady–state or dynamic behaviour. The interface could be illustrate in Fig. 4.

GAMS—General Algebraic Modeling System (http://www.gams.com/) is another language that could provide as an interface to connect the model with the different solvers. The model of the process could be well described by a linear or

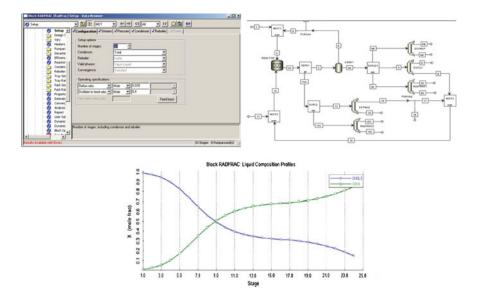


Fig. 3 Aspen Suite interface and results as Process Simulator



Fig. 4 gProms interface and some illustrative outputs

non-linear mathematical formulation using continuous variables (x) and/or discrete/binary ones (y) sometimes called decision variables and transforming the problems in mixed formulation. The generic formulation could be given by considering the optimization direction the minimization as the objective function (f): *Minimise* f(x, y)

Subject to h(x, y) = 0g(x, y) < 0

x Continuous variables $(x_1, x_2, x_3 \dots x_n)$

y Binary variables (y1, y2, y3 ... ym)

As an example of this last approach, are the challenging problems in real world scenarios on the planning and scheduling of the complex oil supply chain. There is a growing need to establish decision support tools capable of dealing with competition within this industry and enable the replacement of simple procedures/tools, such as spreadsheets, with more efficient ones. Relvas et al. (2007) studied a medium term scheduling problem of a pipeline and the associated end-of-pipe tank farm and modelled it as a mixed integer linear problem (MILP). This model represents the articulation between the pipeline schedule and the inventory management at the tank farm. The improvements include variable flowrate, pipeline stoppages, and variable settling period with product. On this scheduling model, a novel rescheduling methodology is developed, taking into account the variability of real plant changes with the definition of revisions of schedules in an effective way. The model and respective rescheduling strategy have been applied to a scenario of a Portuguese oil distribution company. Problems covering one month of time horizon, including initial plans and their revisions, with more than one perturbation, have been successfully solved.

3.2 Methodologies and Tools to Address the Environmental Pillar

The LCA—Life Cycle Assessment is an environmental management tool, which allows the identification and quantification of the environmental impact of a product, process or activity from the extraction of raw materials to the placing as waste in a landfill (cradle to grave). The LCA has been used in numerous industrial sectors such as energy, and today is a well-established methodology with numerous applications in industry, research and decision policies. This methodology is based on four main steps (ISO 14040 2006): (1) Definition of objectives and scope; (2) Life Cycle Inventory; (3) Life Cycle Impact Assessment; (4) Interpretation.

Several methods to evaluate the environmental process impact assessment of industrial chemical processes have been presented in the literature. Although these methods follow the same steps (usually, characterisation, normalisation and weighting), each method addresses different impact categories, considering specific nomenclatures and using different taxonomies to classify their outputs. When

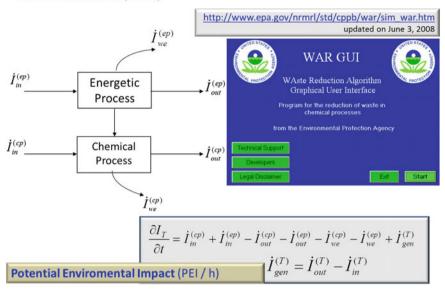


Fig. 5 Methods to carried out LCIA-Life Cycle Impact Assessment

industrial processes are being assessed by several methods, different results are obtained. The comparison of these non-standardised results turns out to be a difficult task. The careful selection of the indicators used in this step should be the subject of a thorough analysis and study (Dewulf and van Langenhove 2006; Carvalho et al. 2014). In Fig. 5 the most relevant methods to carry out LCIA are summarized.

A preliminary study of the different environmental process impact assessment methods revealed important differences in the type of output, namely on the different impact categories. For example, CML method presents 14 midpoint indicators (Heijungs et al. 1992; Guinée et al. 2001), whereas Eco-indicator presents 3 endpoint indicators (Goedkoop and Spriensma 2001), which are combined into a final indicator. For instance, according to the proposed terminology, the ReCiPe method's (Goedkoop et al. 2009) output includes 18 indicators that quantify 18 impact categories, which are designated by the authors as midpoint impact categories/indicators. Another mixed method is the IMPACT 2002+ was introduced by Jolliet et al. in 2003.

The Environmental Analysis processes can also be carried out based on a prospective calculation method of environmental impact (PEI—Potential Environmental Impact), which was introduced by EPA—Environmental Protection Agency (1995). The PEI is a relative measure of the effect that a chemical has potentially on human health and the environment. A mathematical algorithm called WAR-Waste Reduction was developed to determine the value of global PEI process. The result of PEI is a process for calculating a measure of the impact of the



WAste Reduction (WAR)

Fig. 6 WAR-Waste Reduction framework (adapted from Cabezas et al. 1997)

process effluent (Cabezas et al. 1997). The purpose of the application of the methodology is to get the characterization of the process, so that you can make the comparison between possible alternatives (structural and parametric) for minimizing the environmental impact and that will have a direct influence on the choice of alternative leading to a global minimization of effluent. These indices include eight different categories of impacts and can be calculated using the Process Simulation Excel (a first step) and Aspen Plus (a second step).

The eight categories used to calculate the environmental impact potential (PEI) through the WAR algorithm are divide in two groups (Fig. 6): Atmospheric and Toxicological Impacts (Cabezas et al. 1997).

In the group of Atmospheric Impacts four categories could be pointed out:

GWP (Global Warming Potential): measures the absorption capacity of infra-red radiation of a mass unit of a given substance, compared to a mass unit of CO2, over an established time of 100 years.

ODP (Ozone Depletion Potential): compares the reaction rate between a mass unit of a given substance with ozone, and a mass unit of CFC-11 (trichlorofluoromethane) with ozone, to originate molecular oxygen.

PCOP (Photochemical oxidation Potential): compares the reaction rate between a mass unit of a given substance with the hydroxyl radical (OH.), and a mass unit of ethylene with the same radical.

AP (Acidification Potential): quantifies the release rate of H+ in the atmosphere of a given substance, compared to the release rate of H+ due to the formation of SO2.

In the group of Toxicological Impacts four categories could be pointed out:

HTPI (Human Toxicity Potential by Ingestion): based on LD50 for mice (mg of substance/mg of mouse), because most of these values for humans is not available. When LD50 for mice is unknown, estimations are made using molecular methods. HTPE (Human Toxicity by exposure—dermal and inhalation): calculated based on TWA (Time-Weighted Averages) and TLV (Threshold Limit Values) published annually by OSHA, ACGIH and NIOSH.

TTP (Terrestrial Toxicity Potential): It is obtained using the same parameters used to calculate HTPE.

ATP (Aquatic Toxicity Potential): Based on LC50 (similar to LD50) of the aquatic specie Pimephales promelas.

3.3 Methodologies to Address the Social Pillar

The social pillar still comes up with low development in terms of the engineering community, however it can be approached in a pragmatic way, as a strand of health effects and intrinsic safety of processes. For Industrial Processes a special attention is given to Health and Inclusive Design. The human health risk associated with the chemical product is dependent on the speed at which the product is released and the severity of product effects on the environment. The exposure estimation methods can be divided into two classes: Occupational and Community. Occupational exposure occurs at the workplace due to possible use or production of harmful chemicals. The exposure to chemicals can occur by inhalation in the working space, by ingestion of contaminated food or powder, or by direct contact of the substance with the skin or eyes. In Community terms the most common form of exposure is by inhalation of the surrounding air or by direct or indirect use of contaminated water (Allen and Shonnard 2002).

Several Indices could be pointed out to characterise the industrial safety based on different methodologies and indicators:

- Dow Fire and Explosion Index (Dow/AIChE 1987)
- Dow Chemical Exposure Index (Dow/AIChE 1998)
- Mond Index (Tyler 1985)
- Hazop—Hazard and Operability Analysis (CCPS 2009)
- PIIS—Prototype Index of Inherent Safety (Edwards and Lawrence 1993)
- ISI—Inherent Safety Index (Heikkila 1999)
- I2SI—Integrated Inherent Safety Index (Khan and Amyotte 2004)
- PRHI—Process Route Healthiness Index (Hassim and Edwards 2006)

The Inherent Occupational Exposure index (PRHI—Process Route Healthiness Index) was developed to quantify the risk associated to the exposure of workers to industrial processes. This index is influenced by the impact on health due to the potential releases of chemicals (small leaks and fugitive emissions) and the concentration in the air inhaled by workers. The index is calculated based on five indicators:

- ICPHI-Inherent Chemical and Process Hazard Index;
- HHI—Health Hazard Index;
- MHI-Material Harm Index;
- WEC—Worker Exposure Concentration;
- OEL—Occupational Exposure Limit.

Hassim and Edwards (2006) proposed a calculation routine to deliver the various indicators that lead to the calculation of PRHI index.

$$PRHI = ICPHI \times MHI \times HHI \times \frac{WEC_{\max}}{OEL_{\min}}$$

This routine can be applied to cases which present different reaction pathways helping in decision making.

The Inclusive Design is a key approach to obtain an Inherent Safety design (CCPS 2009). It is related to four strategies:

- Minimize: the use of less hazardous substances;
- Replacement for Change: replacing the material by other less dangerous;
- Moderate: carrying out the processes under less dangerous conditions and minimizing the impact in the site if an eventual release of hazardous material or energy occurs;
- **Simplify**: creating simple design facilities in order to reduce complexity and operations mistakes.

For instance to follow the aforementioned **Minimize** strategy, Process Intensification (PI) appears as a possible solution. PI consists of the development of novel apparatuses and techniques that, compared to those commonly used today, are expected to bring dramatic improvements in manufacturing and processing, substantially decreasing equipment-size/production-capacity ratio, energy consumption, or waste production, and ultimately resulting in cheaper, sustainable technologies. Figure 7 shows an example of the minimize strategy by PI of the methylacetate process.

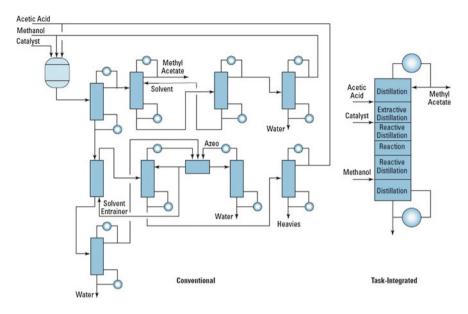


Fig. 7 Example of Inherent Safety design using Process Intensification (drawing courtesy of Eastman Chemical, CCPS 2009)

3.4 Incorporating and Assessing Sustainability in Industrial Processes

Several frameworks have been presented in order to assess sustainability, some at a national level and some at a process level. For instance, General Sustainability Indicators set for the United Kingdom (Defra 2008) consisted of 68 indicators comprising 126 measures covering four major areas: (1) Sustainable consumption and production; (2) Climate change and Energy; (3) Protecting natural resources and enhancing the environment; (4) Creating sustainable communities and a fairer world. In June 2013, based on one consultation it was created a new Sustainable Development Indicators set (SDIs). The new set provides (Defra 2008) an overview of national progress towards a more sustainable economy, society and environment. This SDIs are used as a means of assessing whether the nation as a whole is developing sustainability, and as a means for policy-makers to identify more sustainable policy options. As it can be seen, one of the most critical area in the supply chain is the production, since this entity will influence the four main areas of sustainability at the national level. Therefore, these national frameworks have been adapted to Industrial Analysis. One of the most known specific frameworks are the Sustainable Development Progress Metrics recommended by the Institution of Chemical Engineers for use in Process Industry (IChemE 2007). The three metrics related to the sustainability pillars have some indicators such as: Resource usage (Energy, Raw materials, water, land); Emissions, effluents and waste (atmospheric

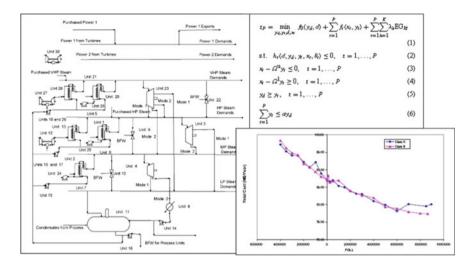


Fig. 8 Utility Network, mathematical model and Pareto Front

impacts, Aquatic impacts and impacts to land); Profit, value and tax (Investments, Additional economic items); Workplace, Society and additional social items.

The previous metrics can be incorporated in the economic models presented in Sect. 3.1, leading to a complete integration of sustainability into process analysis. The balance between the environmental impacts and other economic and social issues leads to multi-objective problems (Young et al. 2000). Pareto front strategy is usually applied to find an integrated process with a clear reduction of environmental impact and to maintain the economic capacity to the required profitability, considering the social effects are not changed. The Pareto front corresponds to a set of solutions where an improvement in one of the objectives can only be achieved by increasing the value of another object. It is a decision support tool for situations where the weights for each objective function or relation between them can be a difficult task (Young and Cabezas 1999; Sikdar and El-Halwagi 2001). An illustrative example is given in Fig. 8 where a utility network is designed assuming the minimization of Total Cost and the reduction of the emissions (Francisco and Matos 2004).

4 Integrated Methodologies

During the past decades several methodologies aiming to analyse sustainability in industrial processes have been presented in the literature. These methodologies have as the ultimate goal the reduction of material consumption, energy, water, environmental and social impacts. These methodologies can be summarized into two types:

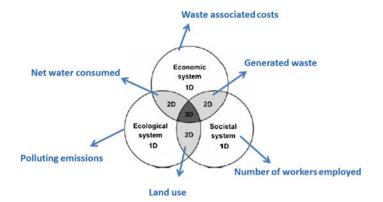


Fig. 9 Example of different dimensions of 3D sustainability analysis (Martins et al. 2007)

- Methodologies integrating sustainability through a set of indicators and aiming to assess process alternatives, helping the decision maker in the choice of the best alternative;
- (ii) Methodologies which evaluate the process in terms of Sustainability, pointing out the critical points and generating new design alternatives. An final assessment is also performed to compare the design alternatives;

The first type of methodologies can be illustrated by the work developed by Martins et al. (2007). This work presents a conceptual structure based on indicators classified in levels, covering three dimensions (3D), two dimensions (2D) and one dimension (1D) indicator. The analysis is performed initially by calculating the 3D windows for different alternatives obtained heuristically and when their analysis have not been conclusive it requires the calculations of other 2D or 1D indicator's (Fig. 9).

The sustainability metric proposed by Martins et al. (2007) for 3D Analysis is based on four indicators:

- **Energy Intensity**: Ratio between the total non-renewable energy consumption and the quantity of produced product;
- Materials Intensity: Ratio between the quantity of raw materials, solvents and other substances and the quantity of produced product;
- **Potential Chemical Risk**: Related to the process dangerousness to the human health due to the use, storage and manipulation of the products;
- **Potential Environmental Impact**: Refers to the environmental impact related to the emissions and discharge of hazardous chemicals to the environment.

The framework proposed to obtain the four indicators has been applied to a simple example of solvent selection, analysing the possibility of replacing the extracting solvent benzene by methyl-n-pentyl ether. The calculations based on process simulation to obtain the energy and materials intensity and safety class tables to obtain the Potential Chemical Risk and Environmental Impact could provide a final result of improvement in all the indicators if the process/solvent alternative is used. The second type of integrated methodologies is illustrated through the methodology developed by Carvalho et al. (2008).

This methodology has been developed for analysing sustainability in industrial processes. The methodology identifies the critical points of the process to change (operating equipment, change materials, etc.). The methodology could guarantee in the end a more sustainable process alternative according to economic, environmental, social and safety issues. The method uses mass and energy indicators, which screen the process, allowing the identification of process bottlenecks, this means the process point that presents mass losses, high costs or undesirable accumulation of species. The indicators that have more severe problems (i.e. high potential for improvement) are selected. A sensitivity analysis to identify target windows, as well as target variables to the desired improvement is performed. The method further involves the use of process synthesis algorithms to suggest new process alternative(s).

The new alternatives are assessed in terms of indicators and metrics. A comparison is carried out between one new alternative and the initial process (base case). In this evaluation metrics for sustainability and security indexes (endpoints) set by IChemE (2007) are used. If the indicators remain constant or improve parameters or, the new alternative is accepted as a more sustainable alternative; otherwise a new process alternative should be assessed and evaluated. This methodology has been incorporated in a software tool, called *SustainPro* (Carvalho et al. 2013). The tool Excel-based has made this methodology a systematic and fast approach to create new sustainable design alternatives. Figure 10 shows the overview of the SustainPro methodology and the usage of different simulations or characterization tools.

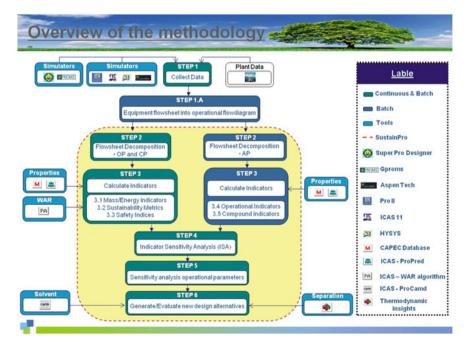


Fig. 10 SustainPro methodology overview with the tools interaction

SustainPro imports input data and performs all the steps of the methodology, as well as the process sustainability assessment for the base case and afterwards for the alternatives. The atmospheric, terrestrial and aquatic impact of the process is determined using the WAR algorithm proposed by the EPA. Social metrics take into account the situation of employees in the workplace, health and safety at the workplace and in society in general. The methodology has been applied to some industrial processes (Carvalho 2009).

One example has been the VCM (vinyl chloride monomer) production The VCM process (PROII 1992) consists in the following sections: (1) Direct chlorination of ethylene. Part of the raw material (1,2-dichloroethane—EDC) is produced by the reaction of ethylene with chlorine; (2) Part of EDC is produced by oxychlorination of ethylene with the recovered acid chloride (HCL) and oxygen; (3) EDC coming from the previous sections and recycled from the process presents approximately 20 compounds as impurities, which should be removed, in a purification process of EDC; (4) Thermal cracking of EDC to form VCM and HCL; (5) VCM's purification.

SustainPro has been applied to the aforementioned process and the most critical areas have been identified. Based on the indicators analysis and on the subsequent sensitive analysis, the recycling of the raw material, turned to be the most critical bottleneck, due to the excess of impurities. SustainPro has applied the synthesis methods, proposing the investment on a membrane, which would be permeable to the impurities, recovering the EDC with a higher purity. The inclusion of this new operation, led to an improvement in the economic pillar (profit increased 0.25 %), in the environmental pillar with the improvement of water and energy metrics (2 %) and finally the social aspects were kept constant, since the safety index has maintained its value from the base case to the new design alternative.

5 Conclusions and Future Work

Sustainability Analysis of Industrial Process is one response of Process Systems Engineering community to the general societal challenge to improve the natural resources usage efficiency. Different approaches of individual characterization of industrial systems (indicators, metrics and ratios) of each of its economic, environmental and social aspects have been properly developed by the scientific community. In a subsequent step, the scientific and technological community elects business areas of engineering knowledge for effective results on the ground of greater equity and sustainability. New methodologies that integrate Sustainability Analysis have been presented, emphasising on new methodologies for identification algorithms or search for critical parts of the process to identify alternatives. These should be characterized in terms of the metrics available so that they can later be recognized as more sustainable alternatives. The presented methodologies and examples point out a positive outlook and constructive approach aimed to generate discussion and develop decision support mechanisms in the conversion of industrial units. There are also job opportunities in the improvement of both the individual techniques for increasing the energy efficiency of processes, either in the development and improvement of new technologies that enable the reduction of energy and/or water consumption. Moreover, two issues still with great potential for research and action for development the integrated methodologies, particularly in the area of operations management and social pillar. The incorporation of knowledge and concepts associated with the vast area of the management of operations. which includes the various methods of obtaining planning and scheduling optimal production should lead to an analysis of wider sustainability. The main goals of this area should be translated into indicators that characterize industrial processes. Their economic and social dimension (e.g. customer satisfaction, increase work efficiency of workers, etc.) should be incorporated into the underlying sustainability metrics for analysis and decision to choose between alternatives. The most intense and deep exploration of the effects on society of certain procedural change or for building integration (e.g. district heating and cooling) can also be further and in this case provides for greater interaction with researchers from the area of sociology. Once developed this aspect, it is supposed that new indicators may be incorporated into the sustainability metrics for complete methodology. Finally, it can be suggested by extrapolation that this approach has some potential to be considered at a macroscopic level of a particular region or country, after the necessary adaptations in the sustainability studies or analysis.

References

- Allen, D. T., & Shonnard, D. R. (2002). Green engineering—Environmentally conscious design of chemical processes. Englewood Cliffs: Prentice Hall.
- Almeida, F. (2007). Os Desafios da Sustentabilidade—uma ruptura urgente. Amsterdam: Campus-Elsevier.
- Brundtland, G. H. (1987). ONU: Our Common Future Report. Acedido em Julho de 2009. http:// www.un-documents.net/wced-ocf.htm
- Cabezas, H., Bare, J. C., & Mallick, S. K. (1997). Pollution prevention with chemical process simulators: The generalized waste reduction (WAR) algorithm. *Computers & Chemical Engineering*, 21, S305–S310.
- Carvalho, A. (2009). Design of sustainable chemical processes: Systematic retrofit analysis generation and evaluation of alternatives. Ph.D. thesis, IST.
- Carvalho, A., Gani, R., & Matos, H. A. (2008). Design of sustainable chemical process: Systematic retrofit analysis and evaluation of alternatives. *Process Safety and Environment Protection*, 86, 328–346.
- Carvalho, A., Matos, H. A., & Gani, R. (2013). SustainPro—A tool for systematic process analysis, generation and evaluation of sustainable design alternatives. *Computers and Chemical Engineer*, 50, 8–27.
- Carvalho, A., Mendes, A. N., Mimoso, A. F., & Matos, H. A. (2014). From a literature review to a framework for environmental impact assessment index. *Journal of Cleaner Production*, 64, 36–62.
- CCPS. (2009). Inherently safer chemical processes: A life cycle approach (2nd ed., p. 411). Wiley-AIChE.

Defra. (2008). The sustainable development indicators in your pocket. Defra Publications.

- Dewulf, J., & van Langenhove, H. (2006). Renewables-based technology: Sustainability assessment. New York: Wiley.
- Dow Chemicals. (1998). Dow's chemical exposure index guide. New York, USA: AIChE.
- Dow Fire & Explosion Index. (1987). Hazard classification guide (6th ed.). Midland, MI: Dow Chemical.
- Edwards, D. W., & Lawrence, D. (1993). Assessing the inherent safety of chemical process routes: Is there a relation between plant costs and inherent safety? *Trans IChemE, Part B, Process Safety and Environmental Protection*, 71(B), 252–258.
- EPA. (1995). Compilation of air pollutant emission factors, Volume I: Stationary point and area sources. Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency.
- Francisco, A. O., & Matos, H. A. (2004). Multiperiod synthesis and operational planning of utility systems with environmental concerns. *Computers & Chemical Engineering*, 28(5), 745–754.
- Goedkoop, M., Heijungs, R., Huijbregts, M., De Schryver, A., Struijs, J., & van Zelm, R. (2009). ReCiPe 2008—A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level.
- Goedkoop, M., & Spriensma, R. (2001). The Eco-indicator 99: A damage oriented method for life cycle impact assessment: Methodology report. Amersfoort: PRé Consultant.
- Guinée, J. B., Gorrée, M., Heijungs, R., Huppes, G., Kleijn, R., Koning, A., et al. (2001). Life cycle assessment: An operational guide to the ISO standards. Centre of Environmental Science, Leiden University, CML.
- Hassim, M. H., & Edwards, D. W. (2006). Development of a methodology for assessing inherent occupational health hazards. *Process Safety and Environmental Protection*, 84(B5), 378–390.
- Heijungs, R., Guinée, J. B., Huppes, G., & Lankreijer, R. M. (1992). Environmental Life Cycle Assessment of Products: Guide. Report 9266, Leiden, The Netherlands: Centre of Environmental Science (CML).
- Heikkila, A.-M. (1999). Inherent safety in process plant design—An index-based approach. Ph.D. thesis, VTT Automation, Espoo, Finland.
- IChemE. (2007). A roadmap for 21st century chemical engineering. Londres: IChemE.
- ISO 14040. (2006). Environmental management—Life cycle assessment—Principles and framework. International Organization of Standardization.
- Jolliet, O., Margni, M., Charles, R., Humbert, S., Payet, J., Rebitzer, G., et al. (2003). IMPACT 2002+: A new life cycle impact assessment methodology. *International Journal of LCA*, 8(6), 324–330.
- Khan, F. I., & Amyotte, P. R. (2004). Integrated Inherent Safety Index (I2SI): A tool for inherent safety evaluation. *Process Safety Process*, 23, 2.
- Martins, A. A., Mata, T. M., Costa, C. A. V., & Sikdar. S. K. (2007). Framework for sustainability metrics. *Industrial & Engineering Chemistry Research*, 46, 2962–2973.
- Meadows, D. H., Meadows, D. L., & Randers, J. (1992). *Beyond the limits*. USA: Chelsea Green Publishing Co.
- Meadows, D. H., Meadows, D. L., Randers, J., & Behrens, III, W. W. (1972). *The limits to growth*. London: Earth Islands.
- OECD. (2012). Material resources, productivity and the environment. www.oecd.org/greengrowth. Accessed in September 2015.
- PRO/II. (1992). Casebook, Simulation Sciences Inc.
- Ramôa Ribeiro, F. (2009). A Energia da Razão- Por uma Sociedade com menos CO2. Gradiva.
- Relvas, S., Matos, H. A., Barbosa-Póvoa, A. P., & Fialho, J. (2007). Reactive scheduling framework for a multiproduct pipeline with inventory management. *Industrial Engineering and Chemistry Research*, 46(17), 5659–5672.
- Sikdar, S. K., & El-Halwagi, M. (2001). *Process design tools for the environment*. London: Taylor & Francis.
- Tyler, B. J. (1985). Using the mond index to measure inherent hazards. *Plant/Operations Progress*, 4(3), 172–175.
- UNFCCC. (2015). http://unfccc.int/2860.php. Accessed in September 2015.

WRI. (2005). http://www.wri.org/our-work. Accessed in September 2015.

- Young, M. D., & Cabezas, H. (1999). Design sustainable processes with simulation: The waste reduction (WAR) algorithm. *Computers & Chemical Engineering*, 23, 1477–2491.
- Young, D., Scharp, R., & Cabezas, H. (2000). The waste reduction (WAR) algorithm: Environmental impacts, energy consumption and engineering economics. *Wast Management*, 20, 605–615.