UNIVERSITAT ROVIRA I VIRGILI
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DESIGN LEVEL:MICROCAPSULES PRODUCTION PROCESS
Jennifer Navarro Rosa
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JENNIFER NAVARRO ROSA

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DOCTORAL THESIS

submitted to the Universitat Rovira i Virgili to fulfil the requirements to obtain the degree of Doctor by the URV

UNIVERSITAT ROVIRA I VIRGILI

Tarragona – Spain
2.009

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Directed by:
Dr. Marta Schuhmacher Ansuategui and Dr. Francesc Castells i Piqué
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CERTIFICAN:

Que presente trabajo, titulado "Framework for Sustainability Assessment of Industrial Processes with Multi-Scale Technology at Design Level: Microcapsules Production Process" que presenta Jennifer Navarro Rosa para la obtención del título de Doctor, ha sido realizado bajo nuestra dirección en el Departament D'Enginyeria Química de esta Universidad y que cumple con los requerimientos para optar al título de Doctora.

Tarragona, 02 de Abril de 2009

Marta Schuhmacher   Francesc Castells

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To my husband and my family

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Abbreviations List

AHP	Analytical Hierarchy Process
CECIF	European Chemical Industry Council
CML	Institute of Environmental Sciences
CV	Contingent Valuation
DALYs	Disability Adjusted Life Years
DSD	Division for Sustainable Development
EHS	Environment, Health and Safety
ELCA	Environmental Life Cycle Assessment
EMA	Environmental Management Accounting
EPA	Environmental Protection Agency
ExternE	External Costs of Energy
FAETP	Freshwater Aquatic Ecotoxicity Potential
GRI	Global Report Initiative
IKP	Institute for Polymer Testing and Polymer Science
IMPULSE	Integrated Multiscale Process Units with Locally Structured Elements
HTP	Human Toxicity Potential
IA	Inventory Analysis
ISO	International Standards Organization
LC	Life Cycle
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCE	Life Cycle Engineering
LCECA	Life Cycle Environmental Cost Analysis
LCIA	Life Cycle Impact Assessment
LCT	Life Cycle Thinking
LCWT	Life Cycle Working Time
LInX	Life Cycle Indexing
LR	Labour Risk
MADM	Multi-Attribute Decision-Making
MAUT	Multi-Attribute Utility Theory
MCA	Multi-Criteria Assessment
MCDA	Multi-Criteria Decision Analysis
MCDSS	Multi-Criteria Decisión Support System
PCE	Perchloroethylene
RIIs	Environmental Resource Impact Indicators
R&D	Research and Development
SAFE	Sustainability Assessment by Fuzzy Evaluation
SD	Sustainable Development
SELCA	Social and Environmental Life Cycle Assessment
SII	Social Impact Indicator
SLCA	Social Life Cycle Assessment
SLCM	Sustainable Life Cycle Management
SUSTECH	Sustainable Chemistry
TAETP	Terrestrial Aquatic Ecotoxicity Potential
TBL	Triple Bottom Line Framework
UN	United Nations
WTP	Willingness-To-Pay

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Publications

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2. Navarro, J., López, E., Castells, F. and Schuhmacher, M. ***Sustainable Life Cycle Management: a case study for selection of soil remediation techniques.*** Oral presentation in International Conference on Life Cycle Assessment. Sao Paulo – Brazil. 26-28 February 2007.

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4. Navarro, J., López, E., Castells, F. and Schuhmacher, M. ***Selecting Soil Remediation Techniques Using Sustainable Life Cycle Management: Methodology and Case Study.*** Poster presentation in 3rd International Conference on Life Cycle Management (LCM). Zurich – Switzerland. 27-29 August 2007.

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"Framework for Sustainability Assessment of Industrial Processes with Multi-Scale Technology at Design Level: Microcapsules Production Process".

Author: Jennifer Navarro Rosa
Directors: Marta Schuhmacher y Francesc Castells

Abstract

The past two hundred years of massive industrialization that started in the middle of the 18th century, with the industrial revolution, showed that productive capabilities of human being could grow exponentially and that labour force was able to manufacture a vastly large volume of basic necessities. This, produced clearly benefits as lower prices, higher incomes and a rapidly raised of standards of living, increasing demand for other products and other industries. But, it also produced the increasing in human population, declining of natural resources, social instability, and environmental degradation; that can be translated in unemployment, illiteracy, poverty, violence, poor nutrition, dangerous machinery and chemicals, noise, pollution, depletion of the ozone layer, global climate change, species extinction, and new diseases, among other concerns. Therefore, the challenge ahead in sustaining life on earth had born and required new vision, with holistic approaches in the development of new environmental benign products and technologies. In a world with limited resources and serious environmental, social and economical impacts, it is obvious that a more sustainable life style is everyday more and more important.

This is where sustainable development was born, which has been defined by the United Nations as development that meets present needs without compromising the ability of future generations to meet their own needs. Sustainable development is based on sustainability, with three pillars of economic, environmental and social.

Due to this, the industrial work has changed from only being reactive in response to governmental legislation, to becoming proactive with the objective to strive towards a more sustainable product family and company to meet future market requirements and opportunities. During the past 30 years, the chemical industry has undergone significant changes and modifications of plants and process integration. As process impacts depend on its structure and design characteristics, its impacts must be considered and minimized at an early stage of process design. Thus, process design started to have an important role in the industry, and nowadays, it aims at creating an

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economic, safe, and environmentally benign process throughout the whole life-time of the plant.

All this has resulted in that new projects are born every day with the main objective of developing new sustainable technologies, processes and products. This is the case of the European's Integrated Multi-scale Process Units with Locally Structured Elements (IMPULSE), where different research groups of the European Union and several groups of the University Rovira i Virgili (URV) are participating. The project aims at effective, targeted integration of innovative micro-structured process equipment, to attain radical performance enhancement for whole process systems in chemical and pharmaceutical production, thereby contributing to significant improvement in supply-chain sustainability for the chemical and pharmacological industry. The IMPULSE approach represents a true paradigm shift in chemical process engineering: Rather than adapting the chemical synthesis routes and process operating parameters to be compatible with equipment limitations, IMPULSE adapts the equipment, structure and process architectures themselves in order to create locally the most desirable conditions for a given physic-chemical transformation. The objective of making production processes in the chemical industry more sustainable is only possible if we have methodologies capable of measuring and comparing the sustainability of processes at design level. One of the IMPULSE subtasks consists of a critical analysis of the advantages and disadvantages of the multi-scale technologies from an environmental, economic and safety/health perspective. In addition to the industry's business arguments, there is also a societal need for such an assessment.

Therefore, the general objective of this work is to develop a methodological procedure for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology at design level.

In order to achieve this goal and to transmit it to future generations, this research work has been embodied in a document divided into 6 chapters:

Chapter 1 provides a brief introduction to the topic with a definition of the problem to investigate, an overview of the existent tools to assess sustainable development, and the setting of the objectives of the research. In this part an exhaustive bibliography review have been made, which is synthesized in the explanation of different existent sustainability assessment methodologies, and in their comparison according to their application level and the sustainability areas (environmental, economic, social, etc.) that they assess. All these methods work with indicators. However, the high number of existent sustainability indicators, their different units and absolute values, make it difficult to interpret and be useful for decision-making purposes. To manage this problem, it is recommended to select a small set of few lead indicators and calculate the combined effect of all categories in the form of a general index of sustainability. Indicators must be chosen for each project according to its specific purposes. To improve sustainability indexes, sensitivity and uncertainty analysis are proposed.

Chapter 2 shows the theoretical bases that were necessary to develop the methodology. Life Cycle Assessment (LCA) is explained in its extension, as well as various concepts associated with environmental, economic, social, eco-efficiency and

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sustainability assessments and management. In addition, the simulation process used in this work are defined and explained in detail

Chapter 3 presents the new developed methodology, called "Sustainable Life Cycle Management" (SLCM). To develop the methodology, the ISO 14040 series for environmental LCA standard has been used as inspiration and followed to the extent since it has proved to be meaningful, practical, besides being international standardized. The new methodology, SLCM, meets the following requirements, which were taken from the ISO 14040 series: the methodology follows the four steps of the ISO 14040 series standards (goal and scope definition, inventory analysis, impact assessment, and interpretation); it allows the analysis of the impacts associated to the product in the three areas of sustainability (economic, environmental, and social) through all stages of the life cycle of the product analyzed (from cradle to grave); it uses a small set of few lead indicators to analyze the impacts; it includes a procedure for the selection of this indicators; it shows the individual results of each indicator; it aggregates the indicators into one overall index; it includes a procedure for sensitivity and uncertainty analysis; and it shows a graphical representation of the results for clear understanding. The methodology is, in general, identical to the ISO 14040 series with the innovation of the integration of the three pillars of sustainability through a process of normalization and weighting based on Analytical Hierarchical Process (AHP), and the graphic presentation of results in a triple bottom line framework which allows seeing the weak points of each technique to compare and improve them if it is appropriate.

The SLCM methodology was implemented in a software application to assess processes with the possibility of comparing different production scenarios. To accomplish this objective, the SLCM methodology was translated to Microsoft® Excel® format followed by a Matlab© programming in order to obtain the sustainability module for MICAP software (developed by IMPULSE partner ETSEQ-URV within T3.2), with the purpose of simulating the "Production of perfume-containing microcapsules" including new multi-scale design technology. MICAP is a deployed simulator that performs the microcapsule synthesis. It is programmed with Mathworks© Matlab© with three different simulation levels: molecular simulation, Computational Fluid Dynamics (CFD) simulation, and process simulation made with the commercial process simulator ASPEN©.

Chapter 4 presents the application of SLCM methodology to the case study "Production of perfume-containing microcapsules" in order to determine the feasibility and data availability, and to compare different process scenarios and parts of the process.

Perfume microcapsules (PMCs) are of great interest to the softener industry as they offer a mechanism for the efficient deposition of perfumes as well as providing long-lasting fragrance benefits. Perfume deposition onto fabrics is an exceptionally inefficient process as over 90 % of perfume added to a softener is lost during washing. Perfumes have to be very fabric substantive and this limits the possible fragrances. Encapsulation of perfume into a microcapsule helps deposition because – with careful control of capsule size – the capsules become entrapped into a fabric during washing and resist being flushed away. The capsules then provide a long-lasting, consumer relevant benefit. At the present PMCs are commercially made using interfacial polymerisation with melamine-formaldehyde (MF). This process happens in bulk and

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takes many hours and uses environmentally unattractive materials (esp. formaldehyde). Capsule robustness is not ideal and storage stability of commercially made MF capsules is mostly marginal.

Therefore, a research group of ETSEQ-URV within T3.2 IMPULSE project had developed a process for production of perfume-containing microcapsules using micro-devices. The description of this production process is explained in the following section. However, as this is an innovative process, it is not possible to compare traditional technology with an intensified process including micro-scale equipment. Thus, a comparison of different scenarios for the same developed process has been made. In this case, two different alternatives for the separation and purification of the final product and the reactives to be recycled are compared by means of the SLCM methodology: Distillation tower separation process (DTSP) and Combined distillation-pervaporation separation process (CDPSP).

Chapter 5 presents the application of the SLCM methodology to a distribution network designed for the product. In this innovative process where micro-equipments are involved, the space used for industrial purpose and the transport of the product between production plants, distribution centers and final seller, will play an important role, and decentralization of industries can be considered as a good option. Thus, in this chapter, a comparison between centralized and dispersed production is analyzed and compared, from the sustainability point of view, also considering different transport types.

Finally in **Chapter 6**, the conclusions chapter presents the conclusions and comes to resume the main features of the model and to propose possible further improvements.

Among the key findings highlighted that the SLCM has shown that it can be used as a decision making tool for sustainability reporting since it integrates the three pillars of sustainability providing an objective criteria for decision making. The case studies analyzed had demonstrated that the methodology can be applied to any process with the same purpose, with the aim of comparing different technologies. In addition, it is clear and easy to follow. The presented SLCM methodology can be applied to any process or activity choosing in each case the corresponding set of inventory data and sustainability impact indicators.

Even when a detailed analysis of the procedure and general and specific data required for the uncertainty calculation, using SLCM methodology, is done in this document; it was not applied to the case studies. Therefore, it is recommended for future works.

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TESIS DOCTORAL:

"Framework for Sustainability Assessment of Industrial Processes with Multi-Scale Technology at Design Level: Microcapsules Production Process".

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Resumen

Los pasados doscientos años de industrialización masiva, empezaron a mediados del siglo XVIII, con la revolución industrial, demostraron que el ser humano es capaz de crecer exponencialmente y que la fuerza laboral es capaz de manufacturar un basto volumen de necesidades básicas. Esto, ha producido claros beneficios como precios bajos, mayores ganancias y un rápido incremento de los estándares de vida, aumentando la demanda de otros productos y de otras industrias. Sin embargo, esto también ha producido el incremento de la población, disminución de los recursos naturales, inestabilidad social y degradación ambiental, lo que puede ser traducido en desempleo, analfabetismo, pobreza, violencia, mala nutrición, maquinarias y químicos peligrosos, ruido, contaminación, deterioro de la capa de ozono, cambio climático, especies en extinción, y nuevas enfermedades, entre otros problemas. Debido a esto, el reto a futuro, de mantener la vida en la tierra ha nacido y requiere una nueva visión, con un enfoque holístico en el desarrollo de nuevos productos y tecnologías ambientalmente benignos. En un mundo con recursos limitados y graves impactos ambientales, sociales y económicos, es evidente que un estilo de vida más sostenible, es cada día más y más importante.

Es aquí donde nace el desarrollo sostenible, que ha sido definido por las Naciones Unidas como el desarrollo que satisface las necesidades del presente, sin comprometer la capacidad de las generaciones futuras para satisfacer sus propias necesidades. El desarrollo sostenible se basa en la sostenibilidad, cuyos tres pilares son el económico, el ambiental y el social.

A raíz de esto, el trabajo industrial ha pasado de ser sólo reactivo en respuesta a las legislaciones gubernamentales, a ser proactivo con el objetivo de avanzar hacia la creación de una familia de productos y empresas más sostenibles para satisfacer las necesidades y oportunidades futuras del mercado. Durante los últimos 30 años, la industria química ha experimentado importantes cambios y modificaciones en plantas y procesos de integración. Como los impactos de los procesos dependen de su estructura y de las características de diseño, los impactos deben ser considerados y minimizados en la fase inicial del proceso de diseño. Por lo tanto, el diseño de procesos comenzó a tener

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un papel importante en la industria, y hoy en día, su objetivo es crear procesos económicos, seguros, y ambientalmente benignos, durante todo el ciclo de vida útil de las plantas.

Todo esto ha traído como consecuencia que cada día nazcan nuevos proyectos con el objetivo principal de desarrollar nuevas tecnologías, procesos y productos sostenibles. Este es el caso del proyecto Europeo IMPULSE (Integrated Multi-scale Process Units with Locally Structured Elements), donde están participando diferentes grupos de investigación de la Unión Europea y de la Universidad Rovira i Virgili (URV). El objetivo de este proyecto es la integración efectiva y eficaz de equipos de proceso micro-estructurados innovadores, con la finalidad de mejorar radicalmente los resultados de los procesos en los sistemas de producción química y farmacéutica, contribuyendo así a una mejora significativa en la cadena de suministro para la sostenibilidad de la industria química y farmacéutica. IMPULSE representa un verdadero cambio de paradigma en la ingeniería de procesos químicos, ya que en lugar de adaptar las rutas de síntesis química y los parámetros de operación de los procesos para que sean compatibles con las limitaciones de los equipos, IMPULSE adapta los equipos, la estructura y la arquitectura de los procesos con el fin de crear, localizadamente, las condiciones más convenientes para una transformación físico-química dada. El objetivo de hacer que los procesos de producción en la industria química sean más sostenibles es posible sólo si tenemos metodologías capaces de medir y comparar la sostenibilidad de dichos procesos a nivel de diseño. De aquí que una de las sub-tareas del proyecto IMPULSE consista en un análisis crítico de las ventajas y desventajas de las tecnologías multi-escala a nivel ambiental, económico y de seguridad / salud.

Por lo expuesto anteriormente, el objetivo general de este trabajo es *"desarrollar un procedimiento metodológico para evaluar la eco-eficiencia y la sostenibilidad de procesos industriales con tecnología multi-escala a nivel de diseño"*.

Con la finalidad de lograr este objetivo y poder transmitirlo a generaciones futuras, el presente trabajo de investigación ha sido plasmado en un documento final dividido en 6 capítulos:

El **Capítulo 1** presenta una breve introducción al tema con la definición del problema a investigar, una visión general de las herramientas existentes para evaluar el desarrollo sostenible, y la definición de los objetivos de la investigación. En esta parte se realiza una revisión bibliográfica exhaustiva, la cual se sintetiza en la explicación de diferentes metodologías de evaluación de sostenibilidad existentes, y en la comparación de las mismas de acuerdo al nivel de aplicaciones y las áreas de la sostenibilidad (ambiental, económico, social, etc.) que evalúan. Todas estas metodologías trabajan con indicadores. Sin embargo, el elevado número de indicadores de sostenibilidad existentes, sus diferentes unidades y valores absolutos, hace que el proceso de interpretación y toma de decisiones resulte difícil. Para gestionar este problema, se recomienda seleccionar un pequeño grupo de indicadores y calcular el efecto combinado de todas las categorías en forma de un índice general de sostenibilidad. Los indicadores deben ser seleccionados para cada proyecto a analizar de acuerdo a los fines específicos del mismo. Para mejorar los índices de sostenibilidad, se propone el uso de análisis de sensibilidad e incertidumbre.

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El **Capítulo 2** muestra las bases teóricas que fueron necesarias para desarrollar la metodología. El Análisis de Ciclo de Vida (ACV) es explicado en su extensión. Así como también diferentes conceptos asociados con la evaluación, análisis y manejo ambiental, económico, social, eco-eficiente, y sostenible. Adicionalmente, se definen y explican en detalle los procesos de simulación utilizados dentro de este trabajo.

El **Capítulo 3** presenta la nueva metodología desarrollada, llamada "Sustainable Life Cycle Management" (SLCM). Para desarrollar esta metodología, la serie ISO 14040 de las normas ISO para el medio ambiente (Análisis de Ciclo de Vida, ACV) han sido utilizadas como inspiración y seguidas en toda su extensión, ya que han demostrado ser útiles y prácticas, además de estar internacionalmente estandarizadas. La nueva metodología, SLCM, cumple con los siguiente requisitos, que fueron tomados de la serie ISO 14040: la metodología sigue los 4 pasos de la serie ISO 14040 (definición de objetivos y alcance, análisis de inventario, evaluación de impactos, e interpretación); permite el análisis de los impactos asociados al producto tanto en las tres áreas de la sostenibilidad (económica, ambiental y social), como en todas las etapas del ciclo de vida del producto analizado (de la cuna a la tumba); utiliza un pequeño conjunto de indicadores importantes para analizar los impactos; incluye un procedimiento para la selección de los indicadores; muestra los resultados individuales de cada indicador; agrega los indicadores en un índice global; incluye la descripción de un procedimiento de análisis de sensibilidad e incertidumbre y muestra los resultados de forma gráfica a fin de facilitar el entendimiento de los mismos. En general, es idéntica a la serie ISO 14040 con la innovación de la integración de los tres pilares de sostenibilidad, mediante un procedimiento de normalización y ponderación basado en el Proceso Analítico Jerárquico (AHP), y la representación grafica de los resultados en un Balance Triple (Triple Bottom Line Framework) que permite ver los puntos débiles de cada tecnología o proceso para compararlo y mejorarlo en caso de que sea conveniente.

La metodología fue implementada en una aplicación de software para evaluar los procesos con la posibilidad de comparar diferentes escenarios de producción. Para lograr este objetivo, la metodología SLCM fue traducida a Microsoft Excel® seguido de una programación en Matlab®, con el fin de obtener el modulo de sostenibilidad del software MICAP (desarrollado por los socios de IMPULSE en T3.2 que son parte de la ETSEQ URV), con el propósito de simular la "producción de micro-cápsulas que contienen perfume" incluyendo la nueva tecnología de diseños multi-escala. MICAP es un simulador de despliegues que simula la síntesis de las micro-cápsulas. Está programado con Mathworks© Matlab© con tres niveles diferentes de simulación: simulación molecular, fluidos dinámicos computacionales (CFD), y simulación de procesos realizada con el simulador de procesos comercial ASPEN©.

En el **Capítulo 4** se presenta la aplicación de la metodología SLCM al caso de estudio de "producción de micro-cápsulas que contienen perfume", a fin de determinar la viabilidad, la disponibilidad de datos, y comparar diferentes escenarios y partes del proceso.

Las micro-cápsulas que contienen perfume (PMC) son de gran interés para la industria de los suavizantes ya que ofrecen un mecanismo eficaz para la deposición de los perfumes y proporcionan el beneficio de una fragancia duradera. La deposición del perfume en los tejidos es un proceso altamente ineficiente, ya que más del 90% del perfume añadido en el suavizante se pierde durante el lavado. La encapsulación de

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perfume ayuda a la deposición del perfume en los tejidos, porque -con un control cuidadoso del tamaño de las micro-cápsulas - éstas se quedan atrapadas en el tejido y se resisten a ser expulsadas fuera del mismo durante el lavado. Posteriormente, las cápsulas proveen a los consumidores, del beneficio de larga duración de la fragancia. En la actualidad las micro-cápsulas con perfume son realizadas comercialmente utilizando la polimerización interfacial con melamina-formaldehído (MF). Este proceso ocurre de forma masiva, tarda muchas horas y usa materiales ecológicamente inatractivos (especialmente el formaldehído). La solidez de las cápsulas no es la ideal y la estabilidad de almacenamiento de las cápsulas de MF es principalmente marginal.

Debido a esto, dentro del proyecto IMPULSE (socio en T3.2, ETSEQ URV), se ha desarrollado un proceso para la producción de micro-cápsulas que contienen perfume mediante micro-dispositivos. Sin embargo, como este es un proceso innovador, no es posible comparar la nueva tecnología que incluye la intensificación del proceso con equipos a micro-escala con una tecnología tradicional. Por lo tanto, se realizó la comparación de diferentes escenarios para el mismo proceso. En este caso, se analizaron y compararon dos alternativas diferentes para la separación y purificación del producto final y de los reactivos a ser reciclados: el proceso de separación utilizando una torre de destilación (DTSP) y el proceso de separación combinado utilizando destilación-per-evaporación (CDPSP).

El **Capítulo 5** presenta la aplicación de la metodología SLCM a una red de distribución diseñada para el producto. En este innovador proceso en el que existen micro-equipos implicados, el espacio utilizado para fines industriales y el transporte del producto entre las plantas de producción, centros de distribución y vendedor final, juegan un papel importante, y la descentralización de las industrias puede ser considerada como una buena opción. Por lo tanto, en este capítulo se realiza el análisis y comparación entre la producción centralizada y dispersa, desde el punto de vista sostenible, considerando también diferentes tipos de transporte.

Finalmente en el **Capítulo 6**, se presentan las conclusiones y se resaltan las principales características del modelo desarrollado, así como también se proponen posibles mejoras.

Entre las conclusiones más importantes resaltan que la metodología desarrollada, SLCM, ha demostrado que puede ser utilizada como una herramienta de toma de decisiones para la realización de informes de sostenibilidad, ya que integra sus pilares proporcionando un criterio objetivo para la toma de decisiones. Los casos de estudio analizados han demostrado que la metodología puede ser aplicada a diferentes procesos con el mismo propósito, a fin de realizar comparaciones entre diferentes tecnologías. Adicionalmente, es clara y fácil de seguir. Esta metodología puede aplicarse a cualquier proceso seleccionando, en cada caso, la correspondiente serie de datos del inventario de los indicadores de impacto y sostenibilidad.

Aun cuando dentro del documento se muestra un análisis detallado del procedimiento y de los datos generales y específicos necesarios para realizar el análisis y cálculo de sensibilidad e incertidumbre, utilizando la metodología SLCM, éste no se aplica a los casos de estudio y se recomienda para trabajos futuros.

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Chapter 1. General Introduction and Background

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1. Introduction

The past two hundred years of massive industrialization that started in the middle of the 18th century, with the industrial revolution, showed that productive capabilities of human being could grow exponentially and that labour force was able to manufacture a vastly large volume of basic necessities. This, produced clearly benefits as lower prices, higher incomes and a rapidly raised of standards of living, increasing demand for other products and other industries (Westkämper et al., 2000). But, it also produced the increasing in human population, declining of natural resources, social instability, and environmental degradation; that can be translated in unemployment, illiteracy, poverty, violence, poor nutrition, dangerous machinery and chemicals, noise, pollution, depletion of the ozone layer, global climate change, species extinction, and new diseases, among other concerns (Andriantiatsaholiniaina et al., 2004). Therefore, the challenge ahead in sustaining life on earth had born and required new vision (Nambiar et al., 2001), with holistic approaches in the development of new environmental benign products and technologies (Kheawhom and Hirao, 2002). In a world with limited resources and serious environmental, social and economical impacts, it is obvious that a more sustainable life style is everyday more and more important (Ljungberg, 2007).

1.1. Sustainability

But it was until 1972, when the environment starts to be an important international issue when the United Nations (UN) first global environmental conference called "Conference on the Human Environment" was celebrated in Stockholm. In that moment, the UN agreed on the urgent need to respond to the problem of environmental deterioration. In 1987, the UN published a report of the World Commission on Environment and Development (the Brundtland Report), entitled "Our common future" (Brundtland, 1987). It developed guiding principles for sustainable development as it is generally understood today and defined the concept as:

"Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs."

The Brundtland report clearly express that the interpretation of the concept could vary from one country to another, but must share the basic concept. In 1992, the UN "Conference on Environment and Development", held in Rio de Janeiro, showed that social, environmental and economic needs must be met in balance with each other since these factors are interdependent and change together. In Rio, the recognition of all Member States of the UN of the need to redirect international and national plans and policies to ensure that all economic decisions fully took into account any environmental impact, end with the Agenda 21 adoption.

In general, sustainability takes into account three aspects, commonly called *three pillars of sustainability* (Figure 1) (Hunkeler, 2006a): 1. Economic: we need economic growth to assure our material welfare; 2. Environmental: we need to minimize environmental damage, pollution, and exhaustion of resources; 3. Social: the world's resources should be shared more equitably between the rich and the poor (Sonnemann et al., 2003).

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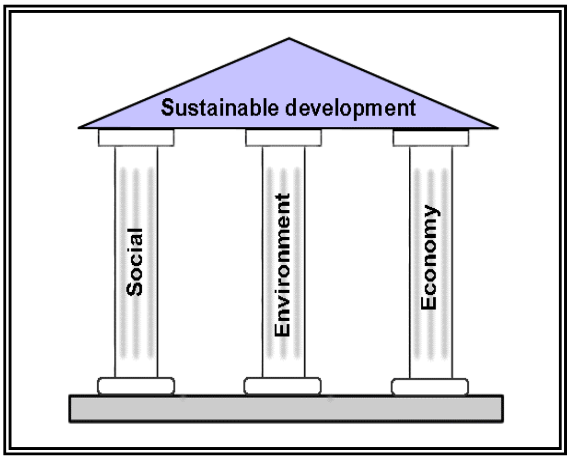

Figure 1. Three Pillars of Sustainability

After 15 years of the Rio Conference, the world is still looking for sustainability and with the pass of the years, the concept has been gained force (Ugwu et al., 2006a), the researches in the area have been increased as the need for more and new sustainable processes (Bovea and Vidal, 2004).

1.2. Designing Sustainable: The IMPULSE Project

Industrial work has changed from only being reactive in response to governmental legislation, to becoming proactive with the objective to strive towards a more sustainable product family and company to meet future market requirements and opportunities (Tingström et al., 2006). During the past 30 years, the chemical industry has undergone significant changes and modifications of plants and process integration (Cziner et al., 2005a). As process impacts depend on its structure and design characteristics, its impacts must be considered and minimized at an early stage of process design (Kheawhom and Hirao, 2002). Thus, process design started to have an important role in the industry, and nowadays, it aims at creating an economic, safe, and environmentally benign process throughout the whole life-time of the plant (Cziner, 2006).

Every day new projects are born with the main objective of developing new sustainable technologies, processes and products. This is the case of the European's Integrated Multi-scale Process Units with Locally Structured Elements (IMPULSE), where different research groups of Euro and several groups of the University Rovira i Virgili (URV) are participating. The project aims at effective, targeted integration of innovative micro-structured process equipment, to attain radical performance enhancement for whole process systems in chemical and pharmaceutical production, thereby contributing to significant improvement in supply-chain sustainability for the chemical and pharmacological industry.

Whereas complete miniaturization or intensification of entire process systems is unrealistic and economically prohibitive, the multi-scale design approach of IMPULSE provides intensification locally only in those parts of a process and on the time and length scale where it is truly needed and can produce the greatest benefit.

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The IMPULSE approach represents a true paradigm shift in chemical process engineering: Rather than adapting the chemical synthesis routes and process operating parameters to be compatible with equipment limitations, IMPULSE adapts the equipment, structure and process architectures themselves in order to create locally the most desirable conditions for a given physic-chemical transformation.

IMPULSE's structured multi-scale design should lead to competitive and eco-efficient chemical production, under locally most desirable conditions. It responds to the need for a knowledge-based manufacturing industry, capable of maintaining substantial production capacity, process and product research, and advanced equipment manufacture in Europe.

IMPULSE goals include the proof of principle in major supply-chain sectors (pharmaceuticals, specialty chemicals, and consumer goods), validated business models (e. g., distributed production, mass customization, etc.), "teachable" generic design methodology and optimization and decision criteria for eco-efficiency.

The objective of making production processes in the chemical industry more sustainable is only possible if we have methodologies capable of measuring and comparing the sustainability of processes at design level. One of the IMPULSE subtasks consists of a critical analysis of the advantages and disadvantages of the multi-scale technologies from an environmental, economic and safety/health perspective. In addition to the industry's business arguments, there is also a societal need for such an assessment.

Sustainability demands fundamental changes in consumption and production patterns. Assessment tools are needed for this evaluation; to gauge whether new multi-scale production process designs contribute to the transition towards sustainable production. Therefore, Life Cycle Thinking (LCT) is at the heart of approaches to assess the relative sustainability properties of alternative processes and to develop more sustainable approaches.

1.3. Life Cycle Thinking (LCT)

"LCT implies that everyone in the whole chain of a product's life cycle, from cradle to grave, has a responsibility and a role to play, taking into account all the relevant external effects. The impacts of all life cycle stages need to be considered comprehensively when taking informed decisions on production and consumption patterns, policies and management strategies." (Toepfer, 2001)

This philosophy has been applied to the environmental field as Life Cycle Assessment (LCA) (Udo de Haes et al., 1999a, 1999b). LCA is an analytical methodology for the systematic evaluation of the environmental aspects of a product or service system through all stages of its life cycle, "cradle to grave" approach (Sonnemann et al., 2003). It examines every stage of life cycle, from raw materials acquisition, through manufacture, distribution, possible use/reuse, recycling and final disposal. It was standardized in 1997, by the International Standards Organization (ISO) in ISO 14040 standards series for LCA (AENOR, 1998, 1999, 2001a, 2001b) and it was updated in 2006 in two standards, ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b).

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For economic area this philosophy has been applied as Life Cycle Costing (LCC) (Senthil et al., 2003). LCC is a discounted cash flow methodology to calculate all monetary inflows and outflows that occur during the life of a system, from the initial capital cost of the system through operation to equipment disposal (Verduzco et al., 2007). The traditional LCC is vaguely defined by the ISO for Building and Construction Assets standard (ISO 15686). Researchers have developed many methodologies that are worldwide used today for different contexts, such as building investments, environment, etc. (Reich, 2005). These methodologies are similar in their approach and structure, but have received different names as: life cycle accounting, life cycle cost assessment, environmental cost accounting, full cost accounting, full cost environmental accounting, total cost accounting, total cost assessment, true cost accounting, etc. (Gluch and Baumann, 2004). Also, different standards exist for LCC as: the Australian Standard for Life-Cycle Costing (AS/NZS 4536:1999), American Society of Testing and Materials standard for Measuring Life-Cycle Costs of Buildings and Building Systems (ASTM E 917-02), etc.

For social area, the researches on this philosophy are still at an early stage and publications on the subject are quite limited (Norris, 2006). Nevertheless, in the last years a lot of research had been dedicated to this area as can be seen i.e. in the Society of Environmental Toxicology and Chemistry (SETAC) North America 27th annual meeting in 2006 where at least ten presentations were dedicated to include the social aspect into LCA framework, as: indicators for social LCA, methodologies and products development including social LCA, combinations of socio-economic and socio-environmental LCA, cases study with social LCA as social label, etc. (SETAC, 2006). The social LCA is about impacts on people and it is a tool to facilitate companies to conduct business in a socially responsible manner. Social LCA have not been standardized until now.

The integration of the three pillars of sustainability had been analyzed by some authors (Klopffer, 2003, 2005; Jasch and Lavicka, 2006; Ny et al., 2006; Schmidt and Butt, 2006; Swarr, 2006; Udo de Haes, 2006). Some authors have been written about the integration of two pillars of sustainability (i.e. economic-environment (Senthil et al., 2003; Gluch and Baumann, 2004; Reich, 2005), environment-social (O`Brien et al., 1996; Yokota et al., 2003; Romero-Hernandez, 2004; Gauthier, 2005)).

However, not all sustainability assessment methodologies are based on LCT. On the following, some sustainability assessment methodologies will be analyzed and the ones meant to assess sustainability at processes design level will be identified latter.

1.4. Sustainability Assessment Methodologies

There are different methodologies for sustainability assessment, that can be used for specific cases according to the level at which the methodologies are applied (products, process, projects, companies, sectors of the economy, cities, countries, etc., see Figure 2) but not necessarily analyzing the complete life cycle of the process or product. LCT is a broader accepted concept but it is also important to analyze methodologies that are not based on this philosophy.

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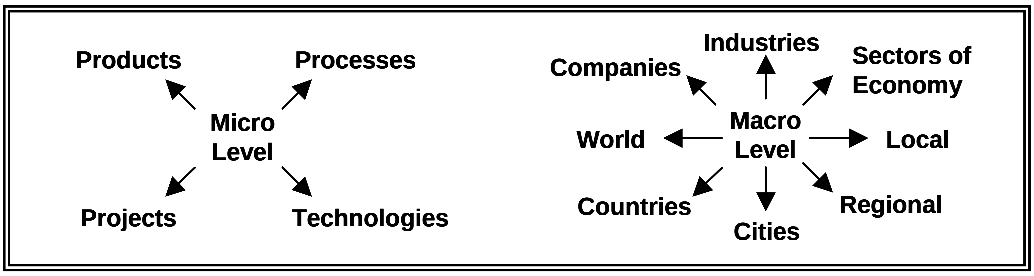

Figure 2. Sustainability Methodologies Application Levels

Table 1 and Table 2 explain sustainability methodologies ordered according to the level at which they are applied, (micro level: products, processes, projects; and macro level: companies, industries, sectors of the economy, cities, countries, world), showing the name of the methodology with a short definition/description, and the sustainability areas (environmental, economic, social, etc.) that the methodology assess; with the only difference that Table 1 shows methodologies **based** on LCT, and Table 2 shows methodologies **not based** on LCT.

On one hand, in Table 1 most of the sustainability assessment methodologies based on LCT analyze one or two sustainability areas. The mix between environment and economic aspects appears to be the most analyzed areas. Few methodologies aim at analyzing the three pillars of sustainability. The social area is the less studied. It looks like there is equilibrium between the number of methodologies that analyze micro and macro levels.

On the other hand, in Table 2 most of the sustainability assessment methodologies that are not based on LCT analyze the three pillars of sustainability, followed by the analysis of a mix between environment and economic aspects. The social area is equally studied as environmental or economic areas. There is an obvious predominance of methodologies that analyze macro levels.

When comparing the information of both tables, methodologies that are not based on LCT, seems to be more complete, since they analyze the three sustainability areas. This could be because LCT is a relatively new philosophy[1], and because methodologies not based on LCT are mostly intended to analyze macro level. The process of translating national strategic sustainability objectives into concrete action at micro (i.e. products/processes) levels remains a difficult task since most of the current initiatives are focussed on macro-level definitions and setting broad-based sustainability goals (Ugwu and Haupt, 2007).

Given the international focus on sustainability in recent years, there is a need for methods and techniques that would facilitate sustainable appraisal and decision-making at micro level in a design stage. But, the literature review revealed that only three methodologies based on LCT philosophy; aim at assessing the three pillars of sustainability at micro level. These three methodologies are: *life cycle sustainability* (Wolf et al., 2001), *life cycle indexing system (LinX)* (Khan et al., 2004), and *the method for process development* (Cziner et al., 2005a; Cziner et al., 2005b; Cziner, 2006) which

[1] LCA was standardized in 1997 and updated in 2006, by the International Standards Organization (ISO).

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is the only one from those three methodologies that analyzes sustainability at micro level in a design stage.

Following, a short explanation of the methodologies based on LCT philosophy that aim at assessing the three pillars of sustainability at micro level is given. *The life cycle sustainability* presented by the Institute for Polymer Testing and Polymer Science (IKP) (Wolf et al., 2001), where indicators are normalized and weight according to countries, but the process is not clearly expressed. *Life cycle indexing system (LinX)* developed by Khan (Khan et al., 2004), includes the subjective weighting and balancing factors based on experts judge and made three procedures of aggregation of indicators that cause error and uncertainty accumulation in the overall index result. *The method for process development* presented by Cziner (Cziner et al., 2005b; Cziner, 2006) which is the only one that makes sustainability analysis at micro level in a design stage.

In the methodology presented by Cziner, 2006, objectives and priority settings are defined at the beginning. A general list of criteria is condensed in a more specific list based on product and process engineering requirements to assess processes using available indicators. Then, alternatives are evaluated based on selected indicators results. The evaluation is based on the assignment of points to each indicator based on a scale from 1 to 5 (1: very bad, 2: bad, 3: neutral, 4: good, and 5: very good). Points obtained from each alternative are summed. The best process is the one that obtained the higher number in the sum. Plenty of contradictions were found when authors tried to combine favourable properties in cases study. Systematic modifications in the processes were proposed with creativity and deep knowledge of chemical engineering science.

It is true that with the pass of the years many methodologies and tools have been applied and developed to planning and measuring sustainable development as a whole or by parts (social, environmental or economic). But in spite of all the efforts that have been done there is still a need for standardized methods and tools that would facilitate sustainability assessment and decision making at micro level in a design stage.

Sustainability assessment tools uses indicators as parameters for measurement of sustainability (Liposcak et al., 2006). There is a high numbers of existent indicators of sustainability which are usually measured in different units and their absolute values are very different (Diaz-Balteiro and Romero, 2004). Therefore, a set of indicators, without any aggregation, is difficult to interpret, cannot provide a concise general overview of system behaviour, and is not useful for decision-making purposes (Kemmler and Spreng, 2007). To manage this problem, it is recommended to select a small sets of few lead indicators and calculate the combined effect of all categories in the form of a general index of sustainability (Afgan and Carvalho, 2004; Krajnc and Glavic, 2005; Afgan et al., 2007).

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Table 1. Sustainability assessment methodologies based on Life Cycle Thinking philosophy

Methodology / Definition	Sustainability Areas
Product level	
Life Cycle Sustainability. It integrates the life cycle working time (LCWT) approach for the most important work-related social issues into the life cycle engineering (LCE) methodology of the Institute for Polymer Testing and Polymer Science (IKP) (Wolf et al., 2001).	- Environmental - Economic - Technical - Social
Life Cycle Environmental Cost Analysis (LCECA). Tool that incorporates costing into the LCA practice (Senthil et al., 2003).	- Environmental - Economic
Model that allows to add value for customer to a product. It is a combination of LCA, LCC, and Contingent Valuation to quantify the customer's value in terms of his/her willingness-to-pay (Bovea and Vidal, 2004).	- Environmental - Economic
Product & Process level	
Life Cycle Indexing System (LInX). It consists in calculate and group indicators at three different levels, applying analytical hierarchical process and composite programming, using weighting and balancing factors based on experts judge (Khan et al., 2004).	- Socio-Political - Technical - Cost - Environment - Resource
Process level	
Combination of LCA and LCC. It combines financial LCC, (which is used in parallel with LCA) and environmental LCC (functioning as a weighting tool) (Reich, 2005).	- Environmental - Economic
Method for Process Development. It is based on the evaluation of available technologies and aiming at new and innovative designs by combining their best features in a creative way (Cziner et al., 2005b; Cziner, 2006).	- Economy and Profitability - Environment - Health & Safety - Quality - Level of Technology
Project level	
True Sustainable Project Life Cycle Management. It integrates project management framework with sustainability principles, showing the need of developing indicators for the social sustainability criteria (Labuschagne and Brent, 2005).	- Environmental - Economic - Social
Company level	
Social Life Cycle Impact Assessment. Methodology to provide information about the potential social impacts on people caused by the activities in the life cycle of their product. The framework is still under development (Dreyer et al., 2005, 2006).	- Social
Industry level	
Social Impact Indicator (SII). It is based on a Life Cycle Impact Assessment (LCIA) calculation procedure for Environmental Resource Impact Indicators (RIIs) (Labuschagne and Brent, 2006).	- Social - Environment
Sectors of Economy level	
Social willingness-to-pay (WTP). It is based on LCA to calculate the environmental impacts of building materials (Wu et al., 2005).	- Environmental - Economic
Social and Environmental Life Cycle Assessment (SELCA). It integrates outcomes of Environmental Life Cycle Assessment (ELCA) and Social Life Cycle Assessment (SLCA) (O`Brien et al., 1996).	- Social - Environmental
Framework for Sustainability Indicators. Tool for performance assessment and improvements for the mining and minerals industry (Azapagic, 2004).	- Environmental - Economic - Social
Country level	
Method for the Identification of Environmental Impact Category Weights. It is based on a panel approach and a Multi-Criteria Decision Aid (MCDA) for use within the weighting step in Life Cycle Impact Assessment (LCIA) (Soares et al., 2006).	- Environmental

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Table 2. Sustainability Assessment methodologies not based on Life Cycle Thinking philosophy

Methodology / Concept	Sustainability Areas
Product level	
Road-map for integration of sustainability issues. Four-phase process for integrating systems and sustainability perspectives into product design, manufacturing, and delivery decisions (Waage, 2007).	- Environmental - Economic - Social
Project level	
Analytical Decision Model and Structured Methodology for Sustainability Appraisal. It uses the "weighted sum model" technique in MCDA and the "additive utility model" in AHP for MCD making, to develop the model from first principles (Ugwu et al., 2006a, 2006b; Ugwu and Haupt, 2007).	- Environmental - Economic - Social - Health & Safety - Resource utilization
Project, Technology & Company level	
Comprehensive Framework of Sustainability Criteria. It assesses sustainability basing weighting values on perception of decision makers, and a combination of monetary valuation and multi-criteria techniques (Labuschagne et al., 2005).	- Environmental - Economic - Social
Company level	
Composite Sustainable Development Index (CSDI). It integrates different indicators using analytical hierarchical process, normalized them, calculated sub-indices, and combined them into the CSDI (Krajnc and Glavic, 2005).	- Economic - Environmental - Societal
Global Reporting Initiative (GRI). It organise "sustainability reporting" in terms of economic, environmental, and social performance (also known as the "triple bottom line") (Moneva et al., 2006).	- Economic - Environmental - Societal
Sectors of Economy level	
Agricultural Sustainability Index. It integrates biophysical, chemical, economic, and social indicators, to measure agricultural sustainability (Nambiar et al., 2001).	- Biophysical - Chemical - Economic - Social
Potential of multi-criteria assessment. It normalizes indicators by sustainability area, assigned weights assuming linear behaviour, applied multi-criteria assessment, and obtained the general index of sustainability. (Afgan and Carvalho, 2004; Liposcak et al., 2006; Afgan et al., 2007).	- Social - Environment - Performance - Market
Overall Sustainability Function. Based on the multi-attribute utility theory (MAUT) to rank Dutch dairy farming systems according to sustainability (Van Calker et al., 2006).	- Environmental - Economic
Index of Sustainability (IS). It aggregates indicators based on distance between outcome and ideal vector. (Diaz-Balteiro and Romero, 2004).	- Environmental - Economic
Local & Regional level	
External Cost of Energy "ExternE" of the European Commission. It evaluates damage costs by the analysis of the impact pathways, and a monetary valuation (Spadaro and Rabl, 2001).	- Environmental - Economic
City level	
Urban Sustainability. It integrates 22 indicators in an index. All the inputs were weighted based on the analytical hierarchy process method and experts consultation (Van Dijk and Mingshun, 2005).	- Economic - Environmental - Societal - Institutional
National level	
Framework for investigating indicator behaviour within policy processes. It argues for the adoption of policy orientation to analyse and design macro-information systems for sustainability (Hezri, 2004).	- Sustainability indicators
Country level	
Triangle Method. To evaluate economic development sustainability. It integrates indicators to calculate indices for sustainability area, and built the triangle (Xu et al., 2006).	- Economic development - Environmental pollution - Resource - Energy Consumption
Energy Indicators System. For tracking sustainability in developing countries, it uses energy based indicators, correlation analysis, and deciles analysis (Kemmler and Spreng, 2007).	- Environmental - Economic - Social

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To calculate a general index of sustainability, some methodologies aggregate the indicators (integrated) and others do not (non-integrated) (Ness et al., 2007). However, as it was explained before, not integrating would not be useful. In the integrated indicators area, some authors used a normalization step followed by a weighting procedure while others used just the second one.

Generally speaking, normalization is to compare to what extent each alternative causes the investigated damage within each impact category and to convert different units into one comparable base. And, weighting is to determine the relative priority of the different impact categories, meaning how important each category is from the perspective of decision makers (Zhou and Schoenung, 2007).

For normalization, two different methods are used: assuming a linear function performance of the indicators' results (Afgan and Carvalho, 2004; Diaz-Balteiro and Romero, 2004; Krajnc and Glavic, 2005; Liposcak et al., 2006; Van Calker et al., 2006; Zhou et al., 2007) and relating the results with the maximum value found (Xu et al., 2006). When assuming a linear function performance of the indicators' results, also different ways are used, as: not relating them to any value or relating them with the maximum value found or with an "ideal" value.

For weighting, four different methods are used. 1) *Panel approach*, were people are asked to judge different categories, as in the Analytic Hierarchy Process (Wu et al., 2005). 2) *Monetization approach*, based on the idea that categories can be measured by money (Wu et al., 2005). 3) *Scenarios approach*, were different weighting scenarios are analyzed (Afgan and Carvalho, 2004; Khan et al., 2004; Afgan et al., 2007), and 4) *Distance-to target approach*, were the weighting factor is the distance from the value to the "sustainable" target (Wu et al., 2005).

The most used normalization procedure is the assumption of linear function performance of the indicators' results, and the most used weighting procedure is the panel approach. However, from the methodologies analyzed in Table 1 and Table 2, only five used both procedures. Three of them were used for sectors of the economy assessment (Liposcak et al., 2006; Van Calker et al., 2006; Zhou et al., 2007), one for company assessment (Krajnc and Glavic, 2005), and one for natural systems assessment (Diaz-Balteiro and Romero, 2004).

2. Formulation of the Problem to Investigate

As it was shown before, there is a need of methodologies to assess and compare sustainability at micro level in a design stage. It is important to note that sustainability refers to the three pillars: economic, environmental, and social.

In the development of such a methodology the ISO 14040 series for environmental LCA standard would be a very good base since they are international standardized and has proved to be meaningful and practical. Nevertheless, some difficulties can be found in the development of this work as the selection of the indicators, the normalization and/or weighting procedure, the uncertainty manage, and the presentation of results, among others.

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It is difficult to select indicators to calculate a general sustainability index because they have to meet certain specific requirements, as: to be relevant, understandable, reliable, scientifically valid, representative, comparable, unambiguous, simple, easy to interpret, etc. and, in aggregate, they should be comprehensive in their coverage of the goals of sustainable development. In general, it is difficult that all of these criteria can be met in practice. Indicators must be chosen for each project according to its specific purposes and trying to meet the most of the criteria mentioned above. However, some general key indicators can be used equally to analyze different projects.

The main problem when aggregating indicators is that grouping cause losses of detailed information and uncertainty accumulation in the overall index result. To improve sustainability indexes, sensitivity and uncertainty analysis can be used. But, most of the sustainability assessment methodologies do not include this area.

Additionally, sustainability indexes are not easy to interpret. It would be useful to graphic the results of the three sustainability areas in the same graphic giving equal importance to each one. The graphic must show with transparency, effectiveness and responsiveness, that the three sustainability dimensions are interdependent and mutually reinforcing. A tool that links these characteristics is the triple bottom line framework which is also a very used tool in sustainability assessments.

The envisaged product is a practical tool, applicable to new technologies (eco-design oriented), easy to calculate and based on generally, reliable and available data. The result will be a set of indicators that can be used directly to elaborate a sustainability report, i.e. GRI report.

3. Objectives of the Investigation

3.1. General Objective

To develop a methodological procedure for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology at design level.

3.2. Specific Objectives

1. To develop a methodological procedure for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology at design level, by:
    a. Identification of key indicators for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology.
    b. Definition of a procedure for selection of indicators.
    c. Definition of models to calculate indicators.
    d. Definition of normalization and weighting procedures.
    e. Definition of a procedure for sensitivity and uncertainty analysis.
    f. Definition of the way to communicate the results

2. To implement developed methodology in a software application.

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3. To analyze the "Production of perfume-containing microcapsules" case study with developed methodological procedure and software, and compare it with different scenarios, by:
    a. Definition of case study and scenarios.
    b. Finding environmental, social and economical information of case study and scenarios.
    c. Application of methodological procedure and software.

4. Structure of the Report

All information obtained in this research has been compiled in the next 6 chapters of this thesis, as it is shown in Figure 3. Chapter 1 presents a short introduction to the topic with a definition of the problem to investigate, an overview of the existent tools to assess sustainable development, and the setting of the objectives of the research. Chapter 2 shows the theoretical bases that were necessary to develop the methodology. Chapter 3 presents the new methodology developed "Sustainable Life Cycle Management". In Chapter 4 & 5 the "Production of perfume-containing microcapsules" and "the design of a product distribution network" are analyzed in detail with the developed methodology. The conclusions, in Chapter 6, come to resume the main features of the model and to propose possible further improvements.

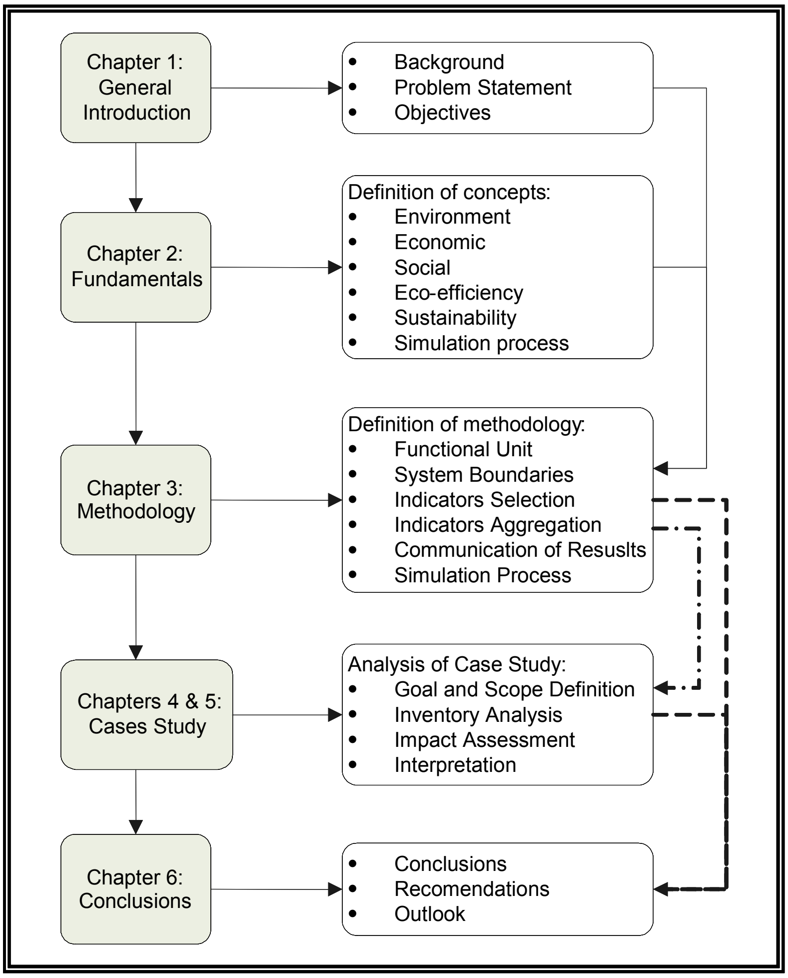

Figure 3. Structure of the Report

UNIVERSITAT ROVIRA I VIRGILI
FRAMEWORK FOR SUSTAINABILITY ASSESSMENT OF INDUSTRIAL PROCESSES WITH MULTI-SCALE TECHNOLOGY AT DESIGN LEVEL:MICROCAPSULES PRODUCTION PROCESS
Jennifer Navarro Rosa
ISBN:978-84-692-4159-2/DL.T-1175-2009

Chapter 2. Fundamentals

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1. Introduction

After exposing that a methodological procedure for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology at design level, had to be developed and implemented in a software application in order to accomplish IMPULSE TB.4 goals, this chapter offers a scheme of the theoretical basis that were used as support for the development of the present investigation. In consequence, “Fundamentals” presents the principal foundations and concepts associated with environmental, economic, social, eco-efficiency and sustainability assessments and management, as well as simulation tools relative to the development of the software application.

2. Environmental Assessments (EA)

Environmental Assessment (EA) is a systematic process that examines the environmental consequences that may result from a proposed or impending intervention. As identified by Environmental Protection Agency (EPA) the overall purpose for undertaking an EA is to seek ways to avoid or minimize adverse effects of a proposed project to the extent practicable, and the maintenance, restoration or enhancement of environmental quality as much as possible (Chowdhury and Amin, 2006).

In the past decade, increasing interest has led to advances in environmental research. Various techniques and methodologies for assessment of environmental performance have been developed to reduce the environmental effects of a variety of products and services (Heikkilä, 2004). Examples include Environmental Impact Assessment (EIA), System of Economic and Environmental Accounting (SEEA), Environmental Auditing, Life-Cycle Assessment (LCA) and Material Flow Analysis (MFA) (Finnveden and Moberg, 2005).

EIA is concerned with the systematic identification and evaluation of the potential impacts (effects), both beneficial and harmful, of proposed projects, plans, programmes or legislative actions related to the physical–chemical, biological, cultural, and socio-economic components of the total environment (Wang et al., 2006). The primary purpose of the EIA process is to encourage the consideration of the environment in planning and decision making and to ultimately arrive at actions which are more environmentally compatible. Numerous EIA methodologies have been developed such as interaction matrices, networks, weighting-scaling (or -ranking or -rating) checklists, multi-criteria/multi-attribute decision analysis (MCDA/MADA), input–output analysis, life cycle assessment (LCA), etc.

2.1. Life Cycle Assessment (LCA)

The first efforts to develop LCA methodology began in the US in the 1970s (Curran, 2006). In 1997, the International Standards Organization (ISO) developed the ISO 14040 series for LCA (Sonnemann et al., 2003) and it was updated in 2006 in two standards, ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b). Moreover, in the

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last years LCA has been a useful tool for the enterprises to provide a framework for identifying and evaluating environmental burdens associated with life cycles of products and/or services they are developing in a "cradle to grave" approach, and to help the enterprises to identify ways to reduce these impacts, and to make cost savings.

"LCA of a product or process comprises the evaluation of the environmental effects produced during its life-cycle, from its origin as a raw material until its end, usually as a waste. This concept goes beyond the classical concept of pollution from the manufacturing steps of a product, taking into account the "upstream" and "downstream" steps" (Sonnemann et al., 2003). Ideally, LCA is applied in a 'cradle to grave' perspective, which implies that the environmental impacts are assessed for the complete life cycle of the product or service, from the extraction of raw materials, through the production process, transport and maintenance, to the disposal stage. An evaluation of a part of the chain is also a possibility, e.g. 'cradle to gate' refers to the production process(es) and all upstream processes. 'Gate to gate' takes into account only the production processes.

LCA methodology is not ready, there are still parts of the methodology that need further attention and development (Bahr, 2004). Moreover, some authors make a call for diversity in LCA methodology and provided a foundation for the consideration of the implications of such methodological diversity as part of an overall approach to promote effective decision making based on LCA environmental performance information (Basson, 2004).

Nevertheless, nowadays a widely accepted methodology is the one standardized by ISO in 1997 and updated in 2006. This methodology is an iterative process that consists of four steps for which ISO series have been developed. Therefore, principles, framework, requirements and guidelines related to each step are written in ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b): goal and scope definition, inventory analysis, impact assessment, and interpretation (Figure 4).

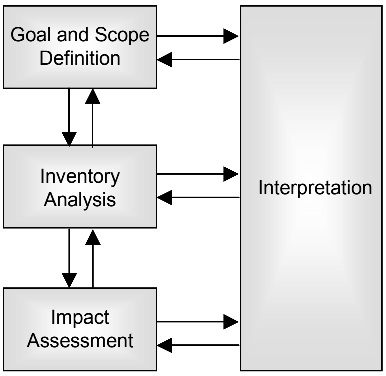

Figure 4. The phases of LCA according to ISO 14040 (2006)

Goal and Scope Definition

In this step an organization of the project is done, is here where the practitioners, stakeholders and the project are defined. Also, more points must be defined in this step: the purpose of the LCA study, the functional unit, the scope of the study (the system boundaries), and a reference flow chart of the process must be drawn (Guinée, 2002).

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- **Functional unit**

The functional unit is the central concept in LCA; it is the measure of the performance delivered by the system under study. This unit is used as a basis for calculation and usually also as a basis for comparison between different systems fulfilling the same function. An example of a functional unit is "the production of 1 kg microcapsules" with, for instance, the aim of comparing the environmental impacts of different industrial production processes of microcapsules.

- **The Systems Boundaries**

The systems boundaries define the range of the system under study and determine the life cycle stages and environmental loads it comprises (Figure 5), and the geographical area where the study is applied.

LCA can be carried out considering the entire list of inputs and outputs (total LCA) or taking into account part of the emissions (partial LCA). In Figure 5, partial LCA 1 considers only raw material and air emissions and is carried out from the beginning (cradle) until gate 3. Partial LCA 2 takes into account only energy losses and noise and goes from gate 3 to the end of life (grave).

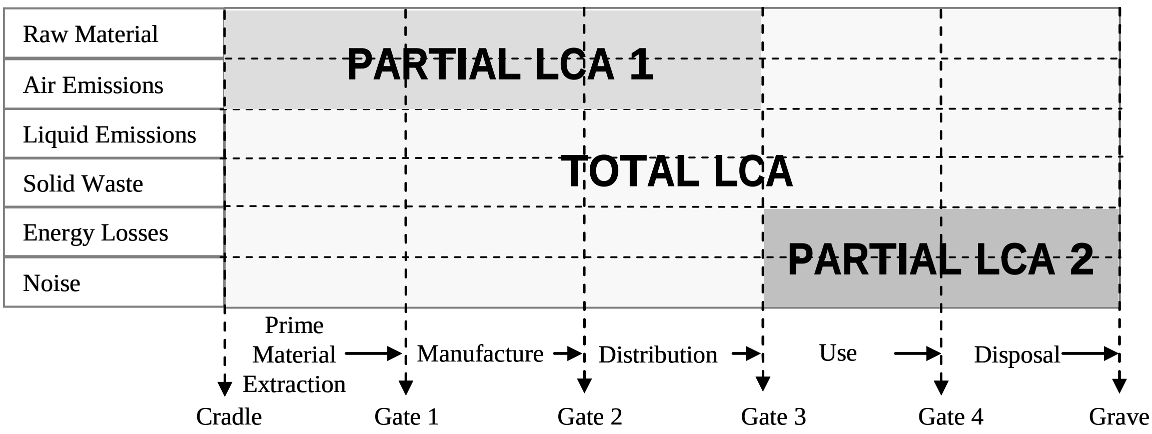

Figure 5. Life Cycle Boundaries

- **Life-Cycle Boundaries**

However, it is often necessary to break life cycle into each of the major life cycle stages and then into individual process steps or components of a product in order to be able to manage the large amount of data generated in a systematic and structured way. This means it is often necessary to use a "gate to gate" approach, such as prime material extraction, manufacturing, distribution, use and waste disposal.

- **Environmental Load Boundaries**

Different types of environmental loads are renewable and non-renewable raw materials, air and liquid emissions, solid waste, energy losses, radiation and noise. LCA can be carried out considering the entire list of inputs and outputs or a partial list.

- **Geographic Boundaries**

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These boundaries refer to the geographic area where the product system to be analyze is located.

Life Cycle Inventory Analysis (LCI)

In the inventory analysis (IA), for each of the product systems considered data are gathered and related to the functional unit of the study (Sonnemann et al., 2003) for all the relevant processes involved in the life cycle. A product system can be considered as a combination of processes needed for the functioning of a product or service. The following steps must be taken (Juraske, 2007):

- **Data collection**

It includes the specification of all input and output flows of the processes of the product system, both product flows (i.e. flows to other unit processes) and elementary flows (from and to the environment).

- **Normalisation to the functional unit**

It means that all data collected are quantitatively related to one quantitative output of the product system under study, most typically 1 kg of material is chosen, but often other units like a car or 1 km of mobility are preferable.

- **Allocation**

It means the distribution of the emissions and resource extractions of a given process over the different functions which such a process.

- **Data evaluation**

It involves a quality assessment of the data, e.g. by performing sensitivity analysis.

The outcome[2] of the inventory analysis is a list of all extractions of resources and emissions of substances caused by the functional unit for every product system considered, generally disregarding place and time of the extractions and releases (Huijbregts, 2001).

Life Cycle Impact Assessment (LCIA)

LCIA aims to improve the understanding of the inventory result. Firstly, it is determined which extractions and emissions contribute to which impact categories. Therefore, the impact calculation methods retained for the study must be chosen, as well as the flows to be taken into account for the calculation of impacts, the impacts have to be calculated, and the principal flows contributing to these impacts must be identified. An impact category can be defined as “a class representing environmental issues of concern to which life cycle inventory analysis results may be assigned” (ISO, 2006a). Consequently, in this step the practitioner has to select and define impact categories, classify, characterize, and the optional elements proposed by ISO are normalized and grouped. In addition, ISO 14044 (ISO, 2006b) includes weighting in the optional elements.

[2] Generally called Life Cycle Inventory.

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- **Selection and definition of impact categories**

In a LCIA, essentially two methods are followed, as shown in Figure 6: problem-oriented methods (midpoint categories) and damage-oriented methods (endpoint categories).

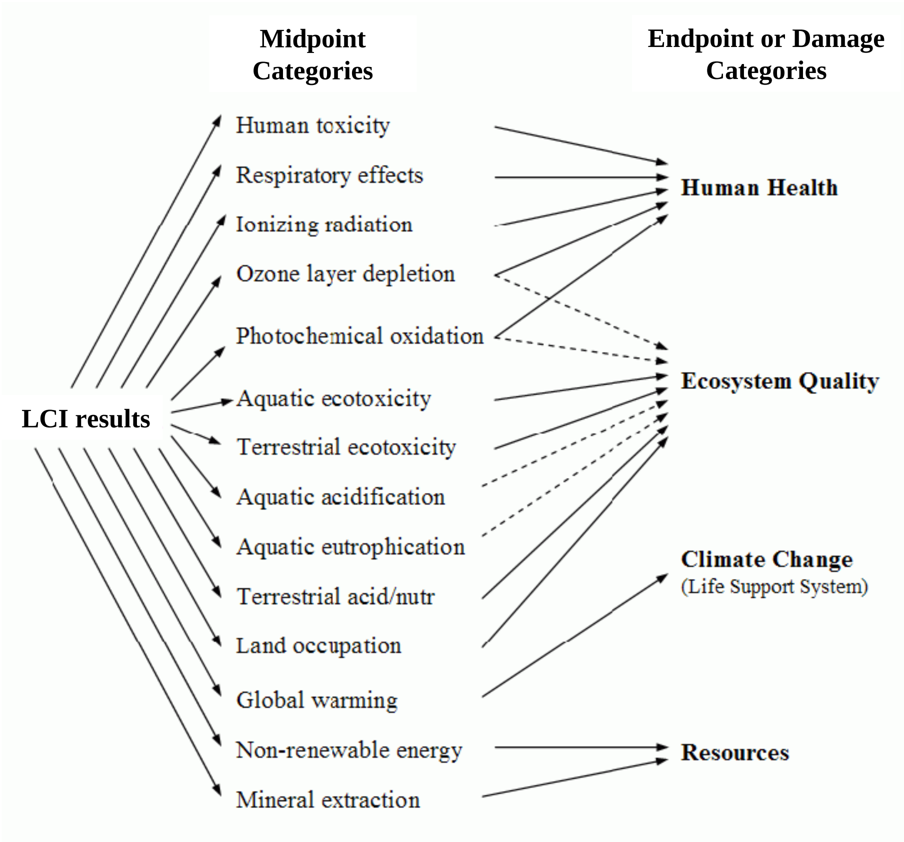

Figure 6. Overall scheme of the LCIA framework, linking Life Cycle Impact (LCI) results via the midpoint categories to endpoint categories (Juraske, 2007)

In the problem-oriented approaches, flows are classified into environmental themes to which they contribute. Themes covered in most LCA studies are: Greenhouse effect (or climate change), Natural resource depletion, Stratospheric ozone depletion, Acidification, Photochemical ozone creation, Eutrophication, Human toxicity and Aquatic toxicity. These methods aim at simplifying the complexity of hundreds of flows into a few environmental areas of interest. The EDIP (Environmental Development of Industrial Products) (Hauschild and Potting, 2004) or CML 2001 (Guinée, 2002) methods are examples of problem-oriented methods.

The damage-oriented methods also start by classifying a system's flows into various environmental themes, but model each environmental theme's damage to human health, ecosystem health, climate change or damage to resources. For example, acidification - often related to acid rain - may cause damage to ecosystems (e.g., in the Black Forest in Germany), but also to buildings or monuments.

Problem-oriented methodologies are based on internationally and scientifically accepted approaches, as ISO 14040 standards, when possible. But some categories, such as human toxicity or aquatic toxicity, remain difficult to model and are currently under

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development and require careful evaluation when used. Even more difficulties with scientific relevance exist with damage-oriented methods, hence careful evaluation is necessary.

An important issue with damage-oriented methodologies is the communication aspect of the results. For example, the human health indicator for EcoIndicator 99 (damage-oriented method) uses the concept of "Disability Adjusted Life Years (DALY)". When assessing the life cycle of drinking water production, how do you communicate that producing drinking water constitutes a certain number of Disability Adjusted Life Years?

An indicator defined closer to the environmental intervention will result in more certain modelling. Midpoint indicators provide more detailed information of which way and in what point the environment is affected. While endpoint indicators (damage oriented) are variables that affect directly the society, midpoint indicators (problem oriented) have a closer relation to the technological and organisational solutions of environmental problems.

There are several methodologies for both methods. The CML 2001 or EDIP methods are examples of problem-oriented methods, as the Eco-Indicator 99 is an example of a damage-oriented method. Some of the existing methodologies are shortly presented in Annex 1 and compared in Annex 2. Environmental indicators based on LCA can be calculated using any of these methodologies, depending on the user preferences and the goal and scope of the project.

Nevertheless, a widely accepted and used methodology is CML 2001 which is based on the ISO Standards for LCA and it presents the different ISO elements and requirements made operational for each step. This methodology provides a list of impact assessment categories grouped into: A: Obligatory or Baseline impact categories, B: Additional impact categories, and C: Other impact categories. For definition of each impact category, see Annex 3. Impact categories related to Groups A, B and C of the CML 2001 methodology). For all the expressed above, this methodology will be used in this work.

- **Classification**

The classification is a qualitative step in which the different inputs and outputs of the system are assigned to different impact categories based on the expected type of impacts on the environment, called areas of protection. The main purpose of the activity is to briefly describe which potential environmental effects the inputs and outputs may cause. The major categories of impacts that should be considered according to the areas of protection are: human health, man-made environment, natural environment, and natural resources. Figure 7 shows a classification for CML 2001 baseline impact categories.

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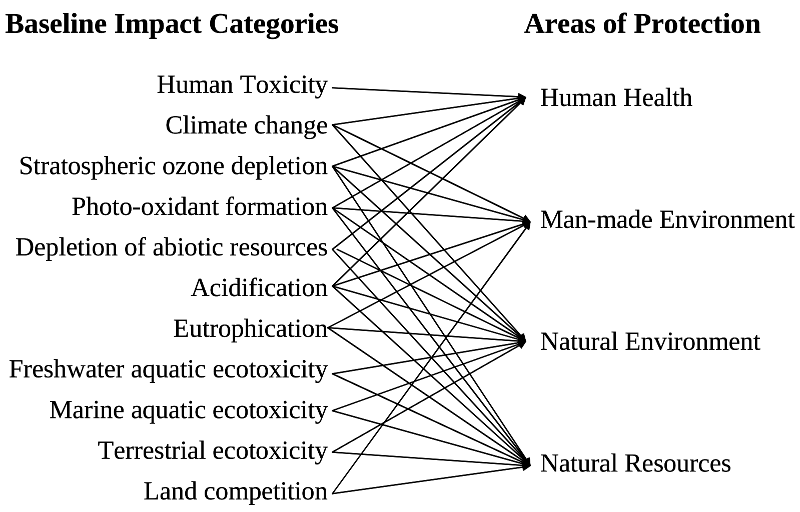

Figure 7. Classification of CML 2001 Baseline Impact Categories

- **Characterization**

In the characterization step the impact categories have to be quantified in terms of a common unit for that category, allowing aggregation into a single score: the indicator result. The resulting figure for one particular impact category is referred to as a category indicator result, and the complete set of category indicator results as the environmental profile.

The environmental profile is calculated by multiplying the interventions of inventory results by their corresponding characterization factors and aggregating the results of these multiplications for each impact category, e.g. for climate change, environmental profile can be calculated as follow (Guinée, 2002):

$$\sum_i WGP_{a,i} \times m_i$$

where $WGP_{a,i}$ is the global warming potential for substance i integrated over a years; and m_i is the quantity of substance i emitted. The result of this environmental profile is in units of equivalent kg of carbon dioxide (CO_2).

Annex 4 shows the formulas used by CML 2001 methodology to calculate the complete set of category indicators or environmental profile.

- **Optional elements of LCIA**
    - **Normalization**

In the normalization step, data from the characterization are related to the total magnitude of the given impact category in some given area and time. A normalization step can provide a better basis for discussions of the results. Normalization can be useful to compare different impact results (Guinée, 2002).

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- **Grouping**

The assignation of the impact categories into one or more sets is performed in this step, in order to facilitate the interpretation of the results into specific areas of concern. Typically grouping involves sorting or ranking indicators (Guinée, 2002).

- **Weighting**

Weighting is the process of converting indicator results of different impact categories by using numerical factors based on value-choices (ISO, 2006b). It may include an environmental index by aggregation of the impact categories (Huijbregts, 2001). Weighting factors represent the relative importance of the impact categories involved.

Life Cycle Interpretation

The final phase in an LCA study is the interpretation of the results from the previous three steps, to draw conclusions and to formulate recommendations for decision makers. Three steps are followed for the interpretation of results.

- **Identification**

This step considers the identification of most important results from Inventory Analysis and Impact Assessment.

- **Evaluation**

Evaluation of the study's outcomes, consisting of a number of the following routines: completeness check, sensitivity analysis, uncertainty analysis and consistency check.

- **Conclusions, recommendations and reporting,**

This section must include a definition of the final outcome; a comparison with the original goal of the study; the drawing up of recommendations; procedures for a critical review, and the final reporting of the results.

3. Economical Assessments

Enterprises and people invest in a very wide variety of projects. The objective of an investment is to maximize the value of the invested money (Ross et al., 1999). To make these investments, stakeholders make decisions based on economic evaluations or analysis which looks at the costs and benefits associated with the particular project investment (Urkiaga et al., 2006). The purpose of an economic analysis is to distinguish among potential projects and determine which one should be implemented (Vawda et al., 2003). Lowest life cycle cost (LCC) is the most straightforward and easy-to-interpret measure of economic evaluation (Fuller, 2007). Some other common used methods are the Net Present Value (NPV), the Rate of Return, and Payback period (PP) (Yrigoyen, 2006). They are consistent with the Lowest LCC measure of evaluation if they use the same parameters and length of study period (Fuller, 2007).

UNIVERSITAT ROVIRA I VIRGILI
FRAMEWORK FOR SUSTAINABILITY ASSESSMENT OF INDUSTRIAL PROCESSES WITH MULTI-SCALE TECHNOLOGY AT
DESIGN LEVEL:MICROCAPSULES PRODUCTION PROCESS
Jennifer Navarro Rosa
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3.1. Life Cycle Costing (LCC)

Traditionally, cost planning and control has focused only on capital costs, instead of on the total lifetime costs (Muñoz Ortiz, 2006). Life Cycle Costing (LCC) is an important economic risk evaluation technique, for identifying, quantifying and analysing all costs, initial and ongoing, associated with a project over its expected life (Ballesty and Orlovic, 2004). Properly interpreted, LCC implies a synthesis of costing analysis and engineering design principles employed to develop product and infrastructure systems that satisfy necessary technical requirements (reflecting customer needs) at minimum life cycle cost (Christensen et al., 2005). Thus, in an ideal case, LCC is used to optimise product performance and lifetime cost of ownership (Gluch and Baumann, 2004).

It is usual to find in the literature different terms related to economic life cycle approaches and/or environmental accounting. Table 3 shows an attempt to define the variants of economic life cycle tools that have been developed during the last decade.

After identifying all costs by year and amount and discounting them to present value, they are added to arrive to the total life cycle cost for each alternative. LCC can be represented by:

$$LCC = C_{pw} + M_{pw} + E_{pw} + W_{pw} + X_{pw} - S_{pw}$$

Where *pw* is a subscript indicates the present worth of each factor. *C* is the capital cost and includes the initial capital expense for equipment, system design, system engineering, and installation. This cost is considered as a single payment occurring in the initial year of the project, regardless of how the project is financed. *M* is the operation and maintenance cost, is figured as the sum of yearly scheduled maintenance and operation costs. It includes salaries for operation, inspections, and insurance. *E* is the energy cost, is the sum of the yearly energy costs. *W* is the water cost, is the sum of the yearly water costs. *X* is the external costs including damage prevention, or damage cost, if occurred. *S* is the salvage value of a system, is its net worth in the final year of the lifetime period (it is usual to find in bibliography that salvage value is 15% of original cost) (El-Kordy et al., 2002). Using the cost factors and the final salvage value, the LCC can be calculated for each alternative system.

3.2. Net present value (NPV)

The net present value (NPV) of an investment is the initial cost of the investment discounted to the present value of the future cash flows of the inversion. NPV of a project of *T* periods can be written as follow:

$$NPV = -I_0 + \sum_{i=1}^{T} \frac{C_i}{(1+r)^i}$$

where: $C_i = R_i - I_i$

The initial flow, $-I_0$, is supposed to be negative since it represents an investment cost at the beginning (i=0). C_i are the future cash flows of the investment that represents the

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subtraction of the investments (cash outflows, I_i) from the returns (cash inflows, R_i) in the time period from i to T. T is the life time of project in years. r is the discount rate, typically 3 to 5 %.

Table 3. Tools commonly used for economic life cycle assessment.

Concept	Definition/description
Environmental cost accounting (ECA)	Refers to the addition of environmental cost information into existing cost accounting procedures and/or recognizing embedded environmental costs and allocating them to appropriate products or processes.
Full cost accounting (FCA)	Identifies and quantifies the full range of costs throughout the life cycle of the product, product line, process, service or activity for the purposes of inventory valuation, profitability analysis, and pricing decisions.
Full cost environmental accounting (FCEA)	Same concept as FCA, but highlights the environmental and possibly health and safety elements.
Total cost assessment (TCA) (I)	Long-term, comprehensive financial analysis of the full range of internal costs and saving of an investment.
Total cost accounting (TCA) (II)	Term used as a synonym for either the definition given to FCA or as a synonym for TCA.
True cost accounting (III)	Another synonym for FCA. As defined by USEPA, this term encompasses both private and societal costs, where full cost accounting encompasses costs that affect the bottom line.
Cost-benefit analysis (CBA)	Describes and quantifies the social advantages and disadvantages of a project in monetary units. If benefits exceed costs, the project is accepted, regardless of how costs and benefits are distributed (Kaldor-Hicks criterion).
Cost-effectiveness analysis (CEA)	Determines the least cost option for a predetermined environmental target, or conversely, the option involving the greatest environmental improvement for a given expenditure.
Life cycle accounting (LCA)	Assignment and analysis of product-specific costs within a life cycle framework.
Life cycle cost assessment (LCCA)	Evaluation of life cycle costs of a product, product line, process, system or facility by identifying environmental consequences and assigning monetary value to these consequences. LCCA is a term that highlights the costing aspect of life cycle assessment (LCA)[3].
Life cycle costing (LCC)	Summing up total costs of a product, process or activity discounted over its lifetime.
Full cost pricing (FCP)	Term used as a synonym for FCA or LCC.
Whole life costing (WLC)	Synonym for TCA (I) or LCC. Defined as "the systematic consideration of all relevant costs and revenues associated with the acquisition and ownership of an asset".

Sources: (Gluch and Baumann, 2004; Muñoz Ortiz, 2006)

The NPV rule is: "an investment must be accepted if the NPV is positive and the greater the NPV the more profitable. If the NPV is negative, the investment must be rejected" (Ross et al., 1999).

3.3. Internal Rate of Return (IRR)

The internal rate of return (IRR) is an indicator of the efficiency of an investment, as opposed to NPV, which indicates value or magnitude. IRR is the rate of interest that

[3] Life Cycle Assessment, Life Cycle Analysis (LCA): environmental management tool explained in Chapter 2 section 2.1. Focuses on environmental impacts, not costs.

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equates the NPV of the cash flow payments to zero (Yrigoyen, 2006). IRR of a project of *T* periods can be written as follow:

$$NPV = -I_0 + \sum_{i=1}^{T} \frac{C_i}{(1+IRR)^i} = 0$$

A project that has a discount rate less than the IRR will yield a positive NPV. The higher the discount rate the more the cash flows will be reduced, resulting in a lower NPV of the project. The company will approve any project or investment where the IRR is higher than the cost of capital as the NPV will be greater than zero. The IRR is therefore the maximum allowable discount rate that would yield value considering the cost of capital and risk of the project. For this reason, the IRR is sometimes referred to as a break-even rate of return. It is the rate at which the value of cash outflow equals the value of cash inflow.

The IRR rule is: “a project must be accepted if the IRR is higher than the discounted rate of return. If the IRR is lower than the discounted rate of return, the project must be rejected” (Ross et al., 1999).

3.4. Payback period (PP)

The purpose of calculating payback period (PP) is to determine the period of time required to recovered the capital invested in a project by annual returns (R_i) (Mahmoud and Ibrik, 2006). The PP is an indicator that shows the level of profitability of an investment in relation to time. PP of a project of T periods can be written as follow:

$$PP = \frac{I_0}{\left(\sum_{i=1}^{T} (R_i - I_i)\right) / T}$$

The PP concept holds that all other things being equal, the better investment is the one with the shorter payback period. The PP rule is: “a project must be accepted if the PP is lower than the PP of other projects. If the PP is higher than PP of other projects, the project must be rejected” (Ross et al., 1999).

IRR and PP are indicators that help selecting the best investment, but they have some problems that can be found in the bibliography (Ross et al., 1999). Therefore, a positive NPV is indispensable to apply any of these methods.

4. Social Assessments

Social Assessment is a process for ensuring that development operations (i) are informed by and take into account the key relevant social issues; and (ii) incorporate a participation strategy for involving a wide range of stakeholders (Rietbergen-McCracken and Narayan, 1998).

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There are many social variables that potentially affect the impacts and success of projects and policies—such as gender, age, language, displacement, and socioeconomic status. Social variables point to measurable change in human population, communities, and social relationships resulting from a development project or policy change (ICGPSIA, 1994). Social assessments need to be selective and strategic, focusing only on those variables of operational relevance.

The social analysis component of a typical social assessment investigates one or more of the following issues: demographic factors, socioeconomic determinants, social organization, socio-political context, needs and values. With this information, social assessment helps project planners assess the social impact of investments and, where adverse impacts are identified, determine how they can be avoided or mitigated (ICGPSIA, 1994).

Social Assessment was developed as a tool for project planners to understand how people will affect, and be affected by, development interventions. It is carried out in order to identify key stakeholders and establish an appropriate framework for their participation in project selection, design, implementation, monitoring, and evaluation. Social Assessment also aims to ensure that project objectives and incentives for change are acceptable to the range of people who are intended to benefit from the intervention, and that project viability and risks are assessed early (Rietbergen-McCracken and Narayan, 1998).

4.1. Social Life Cycle Assessment (SLCA)

SLCA have been the weakest area of sustainability in LCA. Research carried out in this area are still in an early stage and publications on the subject are quite limited (Dreyer et al., 2005, 2006). To mention some works in the social area within LCA framework, one might consider the early “Social and Environmental Life Cycle Assessment (SELCA)” (O`Brien et al., 1996), the development of the Life Cycle Working Time (LCWT) that ends in the well-known GaBi software (Wolf et al., 2001) (see Table 4), and the evaluation of company labour situation based on LCA (Casado Cañeque, 2002) (see Table 4). More recent researches includes two frameworks for social LCA developed in 2006 (Dreyer et al., 2005, 2006; Hunkeler, 2006b).

It is clear that the assessment of the social aspects of all elements of the life cycle is critical future issue for life cycle approaches in general (Hunkeler, 2006a). Nevertheless, there is no standardization of social LCA until today.

4.2. Social Indicators

It is usual to find in the literature different indicators related to social assessment. Table 4 shows common indicators of three different methodologies that have been developed for social assessment in industries. In this table can be seen that it is usual to find health and safety at work within social indicators.

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Table 4. Common indicators used for social assessments in industries.

No.	Theme		Indicator
1	Workplace	Employment situation	• Benefits as percentage of payroll expense • Employee turnover • Promotion rate • Working hours lost as percent of total hours worked • Income + benefit ratio
		Health and safety at work	• Lost time accident frequency • Expenditure on illness and accident prevention/payroll expense
	Society		• Number of external stakeholder meetings per unit value added • Indirect community benefit per unit value added • Number of complaints per unit value added • Number of legal actions per unit value added
2	Qualified working time (QWT)		• Duration of work • Qualification profile of work • Training/Qualification on the job
	Humanity of working time (HWT)		• Worst forms of child labour • Child labour • Forced labour • Discrimination • Equal remuneration for men and women • Share of women work • Right to organise in trade unions • Right to collectively bargain
	Health and Safety of working time (HSWT)		• Lethal accidents • Non-lethal accidents • Heaviness of work
3	Education and training		• Investment in education per worker • Investment in training per worker
	Remuneration		• Remuneration per fixed employ • Remuneration per temporal employ • Remuneration of the administration
	Security		• Incidence ratio • Incidence ratio of lost working days
	Gender		• % of women in the directors associates group • % of women in the directive committee • % of women in the group of managers and directors • % of women into the 25 best paid employees group • % of women in the enterprise
	Diversity		• % of ethnic minorities in the directors associates group • % of ethnic minorities in the directive committee • % of ethnic minorities in the group of managers and directors • % of ethnic minorities into the 25 best paid employees group • % of ethnic minorities in the enterprise

Sources: 1 (IChemE., 2001), **2** (Wolf et al., 2001), **3** (Casado Cañeque, 2002)

4.3. Health and Safety Assessments

In health and safety assessment some usual and easy-to-calculate indicators are the ones related to accidents at work. This is because most of the existing safety analysis methods have been focussed on existing plants or later design phases, where most of the process engineering details are known. These methods cannot be used during the first design phases, since the required detailed information on the equipment and plant layout is missing.

Inherent safety indices were developed for this purpose. They are based on the type of information, which is available early. The safety level of a chemical process can be achieved through inherent (internal) and external means. The inherent safety is related to the intrinsic properties of the inherent safety to remove hazards rather than to controlling them by added-on protective systems, which is the principle of external safety (Hurme and Rahman, 2005). Inherent safety indices usually include the analysis of chemicals, equipment and process characteristics, which are considered as the source of possible accidents at work. These methods are quite fast and reasonably accurate hazard evaluation methods in early process development and conceptual design phases. Table 5 summaries some health and safety analysis tools frequently used in process design.

Inherent safety is used in processes design to choose the “best” from a number of alternative routes, when it is necessary to quantify their inherent safety. Competing routes may be ranked by their index values (lower values indicating that they are inherently safer) in order to identify the one which is potentially the safest and so to aid selection of the route(s) for further development (Heikkilä, 1999; Rahman et al., 2005).

Depending on the case study some of the shown tools can fit better than others to do the analysis, for instance Dow, Mond and FEDI indices are related to storage, handling or processing of flammable, combustible, or reactive material; and TDI to the use of toxic chemicals, while PIIS, ISI, and i-Safe are exclusively related to inherent safety.

According to Rahman et al. (Rahman et al., 2005) inherent safety evaluations can be made in a reasonable accuracy with PIIS, ISI, or i-Safe method. The inaccuracy of indices is related to the differences of their sub-index structure and properties.

In PIIS the evaluation is based on the reaction steps and it does not consider separation sections directly. The reaction hazards are not taken into account directly but through pressure, temperature, physical properties and yields. However, it has the merits of simplicity and therefore it is most straightforward to use. i-Safe includes direct reaction hazard evaluation through heat of reaction and reactivity rating. It does not consider inventory at all neither have direct process equipment related indices. Still the accuracy was not better than with PIIS when analysing cases study. ISI, which has the widest range of indices and therefore it is most elaborate to use, gives the more accurate results. When the process safety ranking is considered, only one method (ISI) gave quite similar ranking to experts. All index methods suffer to some extent from simplifications and lack of sub-index interaction. Despite of their lacks, inherent safety methods are quite fast and reasonably accurate hazard evaluation methods in early process development and conceptual design phases.

In an early phase, inherent safety can be estimated quite well by using the ISI, since most of the information needed is already available. The accuracy of evaluation is nearly as good as in the process pre-design phase coming next. The ISI can give a quite reliable inherent safety ranking of the process alternatives. This index is specifically devoted to inherent safety design and chemical process. It is relevant, transparent, it

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deals with a reasonable number of parameters, the probability of a risk is included to a certain extent, and the quantitative results are clear.

Table 5. Tools frequently used in design level for health and safety analysis.

Concept	Definition/Description
Fire and Explosion Index (F&EI) or Dow Index (Gupta, 1997; Gupta and Edwards, 2003; Gupta et al., 2003)	It purpose is to: quantify the expected damage of potential F&E incidents in realistic terms; identify equipment that would be likely to contribute to the creation or escalation of an incident; determine the areas of greatest loss potential in particular process; and communicate the F&E risk potential to management. F&EI is primarily designed for any operation in which a flammable, combustible, or reactive material is stored, handled, or processed. It primarily covers process units and not complete plants.
The Fire, Explosion and Toxicity Index or Mond Index (Khan and Abbasi, 1998)	The Mond Index is an extension of the Dow Index. The main differences are: to enable a wider range of process and storage installations to be studied; to cover the processing of chemicals which are recognised as having explosive properties; to include a number of additional special process type of hazard considerations to significantly affect the level of hazard; to take into account the toxicity in the risk assessment; to deduce safety distances between the units of a plant; to rank the units according to the level of risk.
The Fire and Explosion Damage Index (FEDI) (Khan et al., 2002)	Estimation of FEDI involves the following steps: classification of the various units in an industry into five categories (storage units, units involving physical operations, units involving chemical reactions, transportation units, and other hazardous units); evaluation of energy factors; assignment of penalties; estimation of damage potential.
Toxic Damage Index (TDI) (Khan et al., 2002)	Toxic damage index (TDI) is a representation of lethal toxic load over an area. It is measured in terms of radius of the area (in meters) getting affected lethally by toxic load (50% probability of causing fatality). This index is derived using transport phenomena and empirical models based on the quantity of chemical(s) involved in the unit, the physical state of the chemical(s), the toxicity of the chemical(s), the operating conditions, and the site characteristics.
Hazard Identification and Ranking (HIRA) (Khan et al., 2002)	HIRA is essentially a combination of two indices: the fire and explosion damage index (FEDI), and the toxicity damage index (TDI)
Prototype Index for Inherent Safety (PIIS) (Edwards and Lawrence, 1993; Rahman et al., 2005)	This index was the first published (in 1993) for evaluating the inherent safety in process pre-design. It is intended for analysing the choice of a process route, i.e. the raw materials used. This method is reaction-step oriented, and it does not consider much the other parts of the process. The PIIS is calculated as a total score, which is a sum of a Chemical and a Process Score. The Chemical Score consist of inventory, flammability, explosiveness and toxicity, and Process Score includes temperature, pressure and yield.
Inherent Safety Index (ISI) (Heikkilä, 1999)	It was developed to take into consideration a larger scope of process steps not only the reaction route but also the separation sections, etc. ISI is a sum of chemical (ICI) and process inherent safety index (IPI). ICI includes chemical reactivity, flammability, explosiveness, toxicity and corrosiveness of the chemical substances present in the process. IPI contains inventory, process temperature and pressure, equipment safety and safe process structure.
i-Safe Index (Palaniappan et al., 2004)	The *i*-Safe Index is called OSI (the Overall Safety Index). It compares process routes by using sub-index values taken from ISI and PIIS plus includes NFPA[4] reactivity rating. It includes mainly the following sub-index: the Individual Chemical Index (ICI) which considers all the properties of the chemicals involved (flammability, toxicity, explosiveness, and NFPA reacting

[4] The National Fire Protection Association (NFPA) system was developed for short-term, often acute exposure to chemicals under conditions of fires or spills. The ratings are intended to provide fire-fighting and evacuation information. It uses a diamond-shaped diagram of symbols and numbers to indicate health, flammability, reactivity/instability and special hazards for many common chemicals.

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	rating; the Individual Reaction Index (IRI) calculated with process parameters (temperature, pressure, yield and heat of reaction); and the Total Reaction Index (TRI) which is the summation of the max of ICI and IRI for each step. Overall Safety Index OSI is the sum of TRIs for each reaction-step and describes the inherent safety of the whole route.

Inherent Safety Index (ISI)

ISI is based on the evaluation of 12 parameters, which are selected to represent major inherent safety factors and are already available in the conceptual design phase. Most of the sub-indices of the method can be estimated quite easily by using physical or chemical properties of compounds present, or based on expected operating conditions that are available from laboratory or pilot plant development work. There is also one sub-index that allows an experience-based evaluation of the safety of the process structure.

ISI is a sum of two main index groups, the chemical inherent safety index (ICI), that describes the chemical aspects of inherent safety; and the process inherent safety index (IPI), that represents the process related aspects. These indices are calculated for each process alternative separately and the results are compared with each other. Table 6 shows the chemical and the process inherent safety indices and its sub-indices.

Table 6. The chemical and process Inherent Safety Index and its sub-indices.

Chemical inherent safety index	Process inherent safety index
Sub-indices for reaction hazards:	*Sub-indices for process condition:*
Heat of the main reaction (I_{RM})	Inventory (I_I)
Heat of side reactions (I_{RS})	Process temperature (I_T)
Chemical interaction (I_{INT})	Process pressure I_P
Sub-indices for hazardous substances:	*Sub-indices for process system:*
Flammability (I_{FL})	Equipment (I_{EQ})
Explosiveness (I_{EX})	Process structure (I_{ST})
Toxicity (I_{TOX})	
Corrosiveness (I_{COR})	

Sources: (Heikkilä, 1999; Rahman et al., 2005)

The ICI contains chemical reactivity, flammability, explosiveness, toxicity and corrosiveness of the chemical substances present in the process. Flammability, explosiveness and toxicity are determined separately for each substance in the process. Chemical reactivity consists of the maximum values of indices for the heats of both main and side reactions, and the maximum value of chemical interaction, which describes the unintended reactions between chemical substances present in the process area studied.

The IPI contains inventory, process temperature and pressure, equipment safety and safe process structure. The index for process structure gives an opportunity to include earlier experience on similar or analogue process concepts in the evaluation. If this sub-index is used, it is to be estimated by an experienced designer or by using case-based reasoning techniques on accident databases.

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Annex 5. Calculation Method for Inherent Safety Index (ISI) shows the calculation procedure for some sub-indices.

5. Eco-efficiency Assessments

The concept of eco-efficiency emerged in the 1990s as a "business link to sustainable development" (Erkko et al., 2005). Many authors have attempted to define eco-efficiency. For example, eco-efficiency means creating more goods and services while using fewer resources and creating less waste and pollution (IISD, 2007). One definition of eco-efficiency that is gaining increasing currency comes from the World Business Council for Sustainable Development (WBCSD):

"Eco-efficiency is achieved by the delivery of competitively-priced goods and services that satisfy human needs and bring quality of life, while progressively reducing ecological impacts and resource intensity throughout the life-cycle to a level at least in line with the earth's estimated carrying capacity" (Verfaillie et al., 2000).

Despite the range of interpretations, note that all definitions have an obvious theme in common; "All concepts call for a more efficient use of natural resources" (Jollands et al., 2004).

Eco-efficiency brings together the two eco dimensions of economy and ecology to relate product or service value to environmental influence (D'Agosto and Kahn Ribeiro, 2004). It can be represented as:

$$Eco-efficiency = \frac{product\ or\ service\ Value}{environmental\ Influence}$$

Progress in eco-efficiency can be achieved by providing more value per unit of environmental influence or unit of resource consumed.

5.1. Eco-efficiency Elements

The WBCSD identified seven elements of eco-efficiency. These elements or characteristics provide a guide to help businesses become more eco-efficient (Côté et al., 2006). They are (Verfaillie et al., 2000):

1. Reduce material intensity.
2. Reduce energy intensity.
3. Reduce dispersion of toxic substances.
4. Enhance recyclability.
5. Maximise use of renewable resources.
6. Extend product durability.
7. Increase service intensity.

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5.2. Eco-efficiency Indicators

The WBCSD recommends generally applicable indicators for measuring and reporting value and environmental performance and additional indicators that are assumed to become generally applicable when standardised measuring methods are developed (Michelsen et al., 2006). The WBCSD recommends the indicators presented in Table 7 as site-specific indicators.

Table 7. Eco-efficiency indicators recommended by WBCSD

Value Indicators	Environmental Influence Indicators
Generally Applicable Indicators	
• **Quantity:** Physical measure or count of product or services produced, delivered or sold to customers. • **Net Sales:** Total recorded sales less sales discounts and sales returns and allowances.	• **Energy Consumption:** Total sum of energy consumed (equals energy purchases minus energy sold to others for their use). • **Material Consumption:** Sum of weight of all materials purchased or obtained from other sources. • **Water Consumption:** Sum of all fresh water purchased from public supply, or obtained from surface or ground water sources (including water for cooling purposes). • **Ozone Depleting Substance (ODS) Emissions:** Amount of ODS emissions to air from processes and losses/replacement from containments (chillers). • **Greenhouse Gas (GHG) Emissions:** Amount of GHG emissions to air from fuel combustion, process reactions and treatment processes, including CO_2, CH_4, N_20, HFCs, PFCs and SF_6 (excluding GHG emissions released in generation of purchased electricity).
Potential Generally Applicable Indicators	
• **Net Profit/Earnings/Income**	• **Acidification Emissions to Air:** Amount of acid gases and acid mists emitted to air (including NH_3, HCl, HF, NO_2, SO_2 and sulphuric acid mists) from fuel combustion, process reactions and treatment processes. • **Total Waste:** Total amount of substances or objects destined for disposal.

Source: (Verfaillie et al., 2000)

6. Sustainability Assessments

As it was explained in Chapter 1 section 1.1, sustainability takes into account three aspects (Sonnemann et al., 2003): economic, environmental, and social. With the past of the years many methodologies and tools have been applied and developed to planning and measuring sustainable development. Some of these methodologies have been already explained in Chapter 1 section 1.4. In spite of all the efforts that have been done there is still a need for standardized methods and tools that would facilitate sustainability assessment and decision making (Bebbington et al., 2007).

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6.1. Use of Indicators

Sustainability assessment tools use indicators as parameters for measurement of sustainability (Liposcak et al., 2006). An indicator represents the measuring parameter for comparison between different states or structure of the system (Afgan and Carvalho, 2004; Afgan et al., 2007; Zhou et al., 2007). Due to the high numbers of existent indicators, these sets are complex, difficult to interpret, and cannot provide a concise general overview of system behaviour (Kemmler and Spreng, 2007). Indicators of sustainability are usually measured in different units and their absolute values are very different (Diaz-Balteiro and Romero, 2004). Therefore, they are not useful for decision-making purposes, because without any aggregation, indicators sets do not provide a measure of progress (Kemmler and Spreng, 2007). It may be useful to use composite sustainable development index, linking many sustainability issues and so reducing the number of options that need to be considerer (Krajnc and Glavic, 2005).

Therefore, to manage the indicators results, the combined effect of all categories under consideration must be express in the form of a general index of sustainability. Selected number of indicators must be taken as a measure of the criteria comprising specific information of the options under consideration (Afgan and Carvalho, 2004; Afgan et al., 2007). For decision-making purposes, less complex frameworks with small sets of a few lead indicators, have more promise (Kemmler and Spreng, 2007).

Independently on the level at which the methodologies are applied, some methodologies aggregate the indicators (integrated) and others do not (non-integrated) (Ness et al., 2007). In the integrated indicators area, some authors used a normalization step followed by a weighting procedure while others used just the second one. A detailed schema to manage the indicators analyzed is shown in Figure 8.

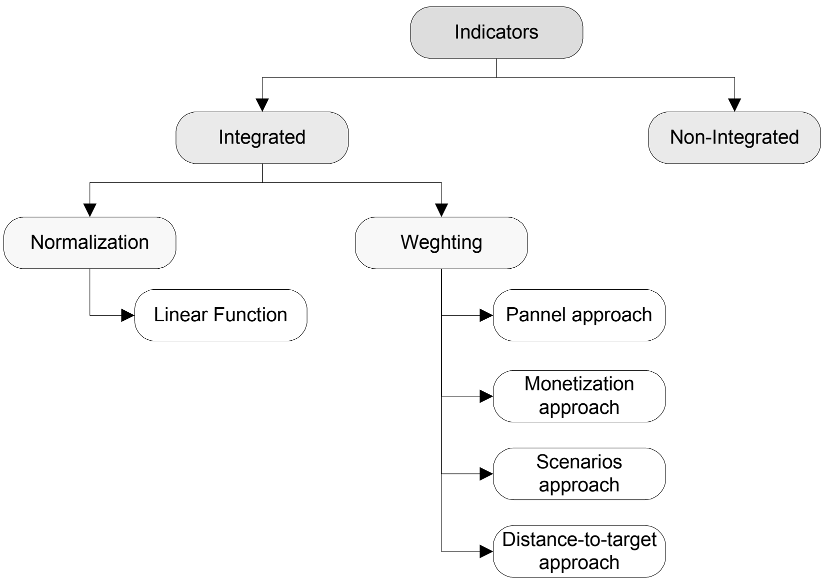

Figure 8. Scheme to Manage Indicators

For normalization, one method is used in different ways. The method is assuming a linear function performance of the indicators' results. In most of the cases, the results are not related with any value (Afgan and Carvalho, 2004; Diaz-Balteiro and Romero,

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2004; Krajnc and Glavic, 2005; Liposcak et al., 2006; Van Calker et al., 2006; Zhou et al., 2007). In other cases, the results are related with the maximum value found or with an "ideal" value (Xu et al., 2006)

For weighting, four different methods are used. 1) *Panel approach*, were people are asked to judge different categories (Wu et al., 2005), like the analytical hierarchical process (Diaz-Balteiro and Romero, 2004; Khan et al., 2004; Krajnc and Glavic, 2005; Labuschagne et al., 2005; Labuschagne and Brent, 2005; Van Dijk and Mingshun, 2005; Cziner, 2006; Liposcak et al., 2006; Ugwu et al., 2006a, 2006b; Van Calker et al., 2006; Xu et al., 2006; Ugwu and Haupt, 2007; Zhou et al., 2007). 2) *Monetization approach*, based on the idea that categories can be measured by money (Wu et al., 2005), are mostly dedicated to integrate only environmental and economical aspects, and they do not use a normalization step (Spadaro and Rabl, 2001; Labuschagne et al., 2005; Labuschagne and Brent, 2005; Reich, 2005; Wu et al., 2005). 3) *Scenarios approach*, were different weighting scenarios are analyzed (Afgan and Carvalho, 2004; Khan et al., 2004; Afgan et al., 2007), and 4) *Distance-to target approach*, were the weighting factor is the distance from the value to the "sustainable" target (Wu et al., 2005), as it was presented in the research of Diaz-Balteiro (Diaz-Balteiro and Romero, 2004).

The most used normalization procedure is the assumption of linear function performance of the indicators' results, and the most used weighting procedure is the panel approach.

The weighting procedure "panel approach" is a multi-criteria assessment, where people are asked to judge seriousness across categories subjectively and empirically through questionnaires or face-to-face communications, and the application is then done in the Delphi or Analytic Hierarchy Process (Wu et al., 2005).

6.2. Multi-Criteria Assessment (MCA)

Multi-Criteria Assessment (MCA) is based on the decision-making procedure reflecting the combined effect of all criteria under consideration and it is expressed in the form of a general index of sustainability (Afgan and Carvalho, 2004; Afgan et al., 2007; Ness et al., 2007; Zhou et al., 2007). Multi-criteria method is very suitable for sustainability assessment (Liposcak et al., 2006). Selected numbers of indicators are taken as a measure of the criteria comprising specific information of the options under consideration. The procedure is aimed to express options property by the respective set of indicators. Therefore, some authors said that multi-criteria assessment do not necessary lead to the best results, since it depends on the priority given to the specific indicators used in the analysis (Zhou et al., 2007). To determine weights of indicators, the evaluators are often confronted with a lack of data. Therefore, the pair-wise comparison technique based on the Analytic Hierarchy Process is used in order to derive relative weights of each indicator practically (Krajnc and Glavic, 2005).

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6.3. Analytic Hierarchy Process (AHP)

The Analytic Hierarchy Process (AHP), developed by Saaty (Saaty and Shang, 2007), is a theory of relative measurement on absolute scales of both tangible and intangible criteria based on paired comparison judgment of knowledgeable experts (Ozdemir and Saaty, 2006).

AHP is a decision making tool intended to help people set priorities and make decision when both qualitative and quantitative aspects of a decision need to be considered (Cziner, 2006). It reduces complex decisions to a series of one-to-one comparisons, then synthesizing the results. The process can be divided into three steps: 1) to perform pair-wise comparison, 2) to assess consistency, 3) to compute the relative weights.

The main advantage of the method is that it measure intangibles working with tangibles to give back measurements to use them in decision making (Ozdemir and Saaty, 2006). Also, it engages decision makers in breaking down a decision into smaller parts and proceeding from the goal to criteria with alternative courses of action (Cziner, 2006). Decision maker can make simple pair-wise comparisons and able to set priorities for certain alternatives. AHP can also measure the degree of inconsistency present in the pair-wise judgments. However, the critics claim that the method gives results that do not necessarily reflect the preferences of the decision maker (Cziner, 2006).

The AHP has been validated with numerous examples in applications that have been published in the literature. These examples are particularly useful for checking on the accuracy of the numbers provided and the numbers derived to validate the process (Ozdemir and Saaty, 2006).

6.4. Triple Bottom Line Framework (TBL)

TBL is used to show sustainability result, and its primary goals are (Mahoney and Potter, 2004):

- Transparency and effectiveness: allowing people to assess or ensure that organizations are doing the right thing in terms of their core business,
- Accountability: allowing organizations to take responsibility for their actions and to report this honestly to their stakeholders,
- Consultation and responsiveness: enabling organizations to ensure positive relationships both internally and externally and responding to the feedback from stakeholders through informed and appropriate decision-making,
- Impact assessment: allowing organizations to identify the nature and scope of impact of the actions they take particularly across and between the three dimensions,
- Information and communication: enabling organizations to use the results of their processes for future decision making and to convey, as and when appropriate, these results to the public.

Under TBL, economic, environmental and social impacts are regarded as being of equal importance. The three dimensions are interdependent and mutually reinforcing. Success is attained through the achievement of overall organizational objectives without compromising the balance of the relationship between the three dimensions (Mahoney and Potter, 2004). The TBL distils a communication focus for complex decision making processes that in reality have to deal with many bottom lines which according to some, currently have too great an emphasis on financial outcomes (Foran et al., 2005).

6.5. Sensitivity and Uncertainty Analysis in Sustainability Assessments

The results of a sustainability assessment are subject to uncertainty due to uncertainty of input data, calculation model and choices made during the study. When comparing several scenarios, it is important to know whether the outcome may be different if one takes into account the uncertainty of data, model and assumptions. In other words, it is important to know whether the results are robust enough to draw clear conclusions. The robustness can be determined by a sensitivity analysis or by an uncertainty assessment.

Sensitivity analysis

Sensitivity analysis plays a fundamental role in decision-making because it determines the effects of a change in a decision parameter on system performance (Andriantiatsaholiniaina et al., 2004). Sensitivity analysis is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation, and how the given model depends upon the information fed into it (Saltelli et al., 2000). The robustness of the results is tested with a limited number of sensitivity checks. To see how the results are affected the check parameters that influence the results are varied, one parameter at a time. The parameter can be, among others, an assumption in the study (e.g. the choice to include or exclude infrastructure data) or a data source (e.g. Ecoinvent) (Rypdal and Flugsrud, 2001).

Uncertainty assessment

The calculation of a sustainability indicator based on life-cycle assessment methodology, may bring about large uncertainties in the indicator score. It is possible that the uncertainty margins in the scores overlap among the alternatives that are compared. In this way, one may no longer be able to discriminate amongst some alternatives, in other words no unambiguous choice can be made which one is best. An uncertainty assessment is useful to get an idea of the total uncertainty of the results, identify the data/factors/choices that contribute most to the uncertainty and the possibilities to improve the reliability of the results (Huijbregts, 2001). An uncertainty analysis aims to quantify the overall uncertainty associated with the response as a result of uncertainties in the model input (Saltelli et al., 2000).

The “uncertainty” referred to above, in fact consists of uncertainty and variability. Uncertainty originates from limitations in translating real world situations into sustainability outcomes, e.g. inaccuracy in measurements, model assumptions or lacking data. Variability is a result of inherent variations in the real world (Heijungs, 2004).

Within an LCA, uncertainty and variability can arise at different levels (Huijbregts, 2001). There are many ways of classifying uncertainty. Table 8 lists a few typologies.

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Reviewing all these typologies, one might ask oneself whether a typology of uncertainties is useful at all. It appears that, no matter how you classify uncertainties, all uncertainties should be dealt with in the appropriate way (Heijungs, 2004).

Table 8. Classification of uncertainty according to several authors.

Bevington & Robinson (1992)	**Morgan & Henrion (1990) Hofstetter (1998)**	**Huijbregts (2001)**
Systematic errors Random errors	Statistical variation Subjective judgment Linguistic imprecision Variability Inherent randomness Disagreement Approximation	Parameter uncertainty Model uncertainty Uncertainty due to choices Spatial variability Temporal variability Variability between sources and objects
Funtowicz & Ravetz (1990)	**Bedford & Cooke (2001)**	**US-EPA (1989)**
Data uncertainty Model uncertainty Completeness uncertainty	Aleatory uncertainty Epistemic uncertainty Parameter uncertainty Data uncertainty Model uncertainty Ambiguity Volitional uncertainty	Scenario uncertainty Parameter uncertainty Model uncertainty

Source: (Huijbregts et al., 2003; Heijungs, 2004; Lloyd and Ries, 2007)

- **Uncertainty of results**

The probability distributions of all inventory data can be combined, to calculate the uncertainty of the indicator score. This can be done by, for instance, Monte Carlo simulation. This takes into account possible correlation among data - for example, the material amount may be related to the energy consumption and the other way round (Heijungs, 2004).

The resulting probability distribution for the indicator score of each option compared can be shown in one figure to indicate whether overlap is occurring, and what is the probability that the conclusions are incorrect.

This procedure mainly covers the parameter uncertainty and, if multiple scenarios are calculated, uncertainty due to choices.

7. Sustainability Assessment Software Tools

Several computerised-aided solutions are currently available for sustainability assessment. Most of these softwares are aimed for analysis at the end of any project stage, i.e. at the end of the process design; only few of them can be applied at early stages. Some methods developed have been reviewed to know the current situation on sustainability assessment software tools. Only some considered representative tools of different application fields have been selected in this analysis, the tools have been divided into three sections:

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- **Fate and transport tools.** These tools help in the development of eco-vector and environmental LCI of products.
- **Life cycle impact assessment tools.** These tools are aimed at helping with the calculation of environmental impacts of products.
- **Full LCA tools.** These tools are capable of calculating the complete LCA of a product. Some of them include the three sustainability areas.

Table 9 compiles the selected solutions, and a brief description is included.

Table 9. Sustainability models and software

Software / Description
Fate & Transport tools
Internet Geographical Exposure Modelling System (IGEMS): brings together several EPA environmental fate and transport models. IGEMS includes models and data for ambient air, surface water, soil, and ground water, and makes the models much easier to use than their stand-alone counterparts.
CalTOX: is a risk assessment model that calculates the emissions of a chemical, the concentration of a chemical in soil, and the risk of an adverse health effect due to a chemical. It consists of two parts: 1. a multimedia environmental fate model, which evaluates the distribution of a chemical among different environmental compartments, and 2. a multiple pathway exposure model, which calculates how much of a chemical reaches the body using environmental concentration and contact factors (e.g. breathing rate).
GLOBOX: is a global multimedia fate, exposure, and effect model, largely based on the EU model EUSES. It has been constructed for the calculation of spatially differentiated LCA characterisation factors on a global scale. GLOBOX consists of three main modules: 1. an impact-category independent fate module; 2. a human-intake module, applicable to all impact categories that are related to humans; 3. an effect module, in which effect-related parameters can be introduced for each impact category.
USES-LCA: is a nested multi-media fate, exposure and effects model for calculating toxicity potentials. It is based on the Uniform System for the Evaluation of Substances, USES, model version 2.0, which has been adapted for the specific demands of the LCA. It calculates the toxicity potentials for six impact categories: aquatic ecotoxicity in fresh water and sea water, ecotoxicity in the sediment of fresh water and sea water, terrestrial ecotoxicity and human toxicity from a possible initial emission from the air, fresh water, sea, agricultural soil and industry soil compartments in Western Europe.
OMNIITOX: is based on the fact that in all types of models of the nature system used in industrial applications causes, effects, and the relation between them within a defined system frame can be identified. In toxic LCIA the focus is on estimating toxic effects caused by emissions from technical systems. In OMNIITOX the focus lays on toxic effects caused by substances in emissions, not LCA of substances in products.
EcoSense: was developed to support the assessment of priority resulting from the exposure to airborne pollutants, namely impacts on health, crops, building materials, forests, and ecosystems. Global warming is not covered by EcoSense. Priority impacts like occupational or public accidents are not included either. It covers 13 pollutants, but does not include impacts from radioactive nuclides.
Life Cycle Impact Assessment tools
IMPACT 2002+: is a life cycle impact assessment methodology that proposes a feasible implementation of a combined midpoint/damage approach, linking all types of life cycle inventory results (elementary flows and other interventions) via 14 midpoint categories to four damage categories.
EDIP97: is a thoroughly documented midpoint approach method covering most of the emission-related impacts, resource use and working environment impacts with normalization based on person equivalents and weighting based on political reduction targets for environmental impacts and working environment impacts, and supply horizon for resources.
Eco-indicator 99: is a “damage oriented” impact assessment method for LCA, with many conceptual breakthroughs. The method is also the basis for the calculation of eco-indicator scores for materials and processes. These scores can be used as a user friendly design for environment tool for designers and product managers to improve products.
Full LCA tools

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SimaPro 7: allows implementing Life Cycle Assessment in a flexible way. The new SimaPro 7 provides a professional tool to collect, analyze and monitor the environmental performance of products and services. It can easily model and analyze complex life cycles in a systematic and transparent way, following the ISO 14040 series recommendations. It includes the different impact assessment methods.
Umberto: visualizes material and energy flow systems. It is a tool for advanced process, flow and cost modelling. With its graphic interface even the most complex structures can be modelled: production facilities in a company, process and value chains and product life cycle.
ECO-it software: allows modeling a complex product and its life cycle in a few minutes. ECO-it calculates the environmental load, and shows which parts of the product's life cycle contribute most. With this information the environmental performance of the product can be improved. ECO-it uses Eco-indicator scores to express the environmental performance of a product's life cycle as a single figure.
Gabi4: provides solutions for different problems regarding cost, environment, social and technical criteria, optimization of processes and managing your external representation in these fields.

Source: (Dreyer et al., 2003; García-Serna et al., 2007; Rosenbaum et al., Submitted)

8. Process Simulation

The process simulation is a tool used to reproduce in a detailed and accurate way the behaviour of processes for its analysis and optimization. The simulations perform the energy and mass balance, predicting operation conditions and stream compositions of the process. Since the results obtained in the simulation are predictions, it is necessary to validate them with experimental data. The process simulation considers the following aspects (Yrigoyen, 2006):

- Definition of thermodynamic and physical-chemical properties
- Description of the involved compounds, reactions and equipment
- Specification of the product or products
- Description of the process by a flow chart
- Equipment sizing

8.1. MICAP simulator

MICAP is a deployed simulator that was developed by IMPULSE partner ETSEQ-URV within T3.2, with the purpose of simulating the "Production of perfume-containing microcapsules"[5] including new multi-scale design technology.

The aim of MICAP is to simulate the microcapsule synthesis. To carry out it, three level simulations have been identified:

- Molecular simulation in order to predict the precipitation of the polymer and thus, the morphology of the microcapsule.
- Computational Fluid Dynamics (CFD) simulation in order to predict the flow dynamics inside the microdevices.
- Process simulation to predict, globally, the synthesis of microcapsules. This simulation was made with the commercial process simulator ASPEN©
- An environmental analysis, which is the second objective of this thesis, must complement the simulator. Therefore, an assessment of eco-efficiency and sustainability of the process is carried out.

[5] Study provided by IMPULSE partner ETSEQ-URV within T3.2 (reported in D3.2c and D3.2f).

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Molecular and CFD simulation are carried out by their own and independently from others. Process simulation is carried out from experimental results and from the molecular and CFD simulation ones. The MICAP simulator performs the microcapsule synthesis process simulation with the microdevices, as a stand-alone application or jointly with a new unit operation created in the ASPEN© commercial process simulator. MICAP simulator has been programmed with Mathworks© Matlab©. It is a deployed application that can be installed in any Microsoft© Windows© platform. Additionally, a new unit operation has been created in ASPEN© which calls the MICAP application, shares data and gets results in order to continue with global simulations in ASPEN©. For sustainability analysis, the SLCM methodology was translated into Microsoft® Excel® format followed by a Matlab© programming in order to obtain the sustainability module for MICAP software.

The execution of this simulator has been carried out by different research groups within IMPULSE consortium at ETSEQ-URV. The different groups are involved in different tasks from the project. Therefore, this work supposes a three-level interaction between: research groups, type of simulations/environmental analysis and project tasks/work-packages (SP3, TB and TC).

8.2. ASPEN PLUS® process simulator

Among the different software solutions designed to help engineers of both university and industry world in processes Aspen Suite is one of the most popular, which covers a wide range of applications. For instance, Aspen HYSYS® and Aspen Plus® for process simulation and optimization, Aspen DMCplus™ for advanced process control, Aspen PIMS™ for advanced planning & scheduling, and Aspen InfoPlus.21™ for plant information management are useful utilities for design within Chemical Engineering. AspenONE includes a full complement of specific software for Oil & Gas, for Petroleum, for Chemicals, for Specially Chemicals, for Consumer Products, for Pharma and for Engineering & Construction. Many of these specific software packages, applied in the right way, may help in the improvement of sustainability techniques for the design of products and processes. These tools should be introduced at early stages of design and included chemical engineering curriculum, so that, future engineers will be able to design towards sustainability (García-Serna et al., 2007).

Aspen Plus® is a market-leading process modelling tool for conceptual design, optimization, and performance monitoring for the chemical, polymer, specialty chemical, metals and minerals, and coal power industries. Aspen Plus is a core element of AspenTech's AspenONE™ Process Engineering applications (AspenTech, 2004).

Process simulation with Aspen Plus® allows to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. Given reliable thermodynamic data, realistic operating conditions, and the rigorous Aspen Plus® equipment models, actual plant behaviour can be simulated. Aspen Plus® can help to design better plants and increase profitability in existing plants.

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With Aspen Plus® the user can interactively change specifications, such as flow sheet configuration, operating conditions, and feed compositions, to run new cases and analyze alternatives. To analyze results, plots, reports, PFD-style drawings, and spreadsheet files can be generated.

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Chapter 3. Methodology

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1. Introduction

In this section, the developed methodological procedure for eco-efficiency and sustainability assessment that put together the economic, environmental and social aspects, of industrial processes with multi-scale technology at design level, based on the ISO 14040 series, is presented.

To develop the methodology, the ISO 14040 series for environmental LCA standard has been used as inspiration and followed to the extent since it has proved to be meaningful and practical. After the analysis of the ISO series some requirements were taken into account for the development of the new methodology. First, the new methodology must follow all the steps of the ISO 14040 series, since it is international standardized. Second, the methodology must allow the analysis of the impacts associated to the product in the three areas of sustainability through all stages of the life cycle of the product analyzed (from cradle to grave). Third, it must use a small set of few lead indicators to analyze the impacts, and the methodology must include a procedure for the selection of this indicators. Fourth, it must show the individual results of each indicator. Fifth, it must aggregate the indicators into one overall index. Sixth, it must include a procedure for sensitivity and uncertainty analysis. Seventh, it must show a graphical representation of the results for clear understanding.

In order to accomplish the third objective of this thesis, the methodology must allow the comparison of different scenarios or different technologies with the same purpose, from a sustainability and eco-efficiency point of view. Therefore, a scenarios description must be included when applying the methodology.

2. Scheme of the Methodology

Based on the above mentioned requirements and after analyzing how to integrate the ISO 14040 framework within the three pillars of sustainability, a scheme for the new methodology, called Sustainable Life Cycle Management (SLCM) was developed, following the four steps of the standard: goal and scope definition, inventory analysis, impact assessment, and interpretation. These steps have to be applied equally for each scenario to be analyzed. Figure 9 shows the new methodology scheme, which is in general identical to the ISO 14040 series with the innovation of the integration of the three pillars of sustainability where a normalization and weighting procedure based on analytical hierarchical process takes place, and the results are presented in a triple bottom line framework which allows seeing the weak points of each technique to compare and improve them if it is appropriate.

3. Goal and Scope Definition

In this step an organization of the project is done, the purpose of the study and the functional unit must be defined, and the system boundaries must be set, for the environmental, economic and social aspects, for each technology to be analyzed and compared.

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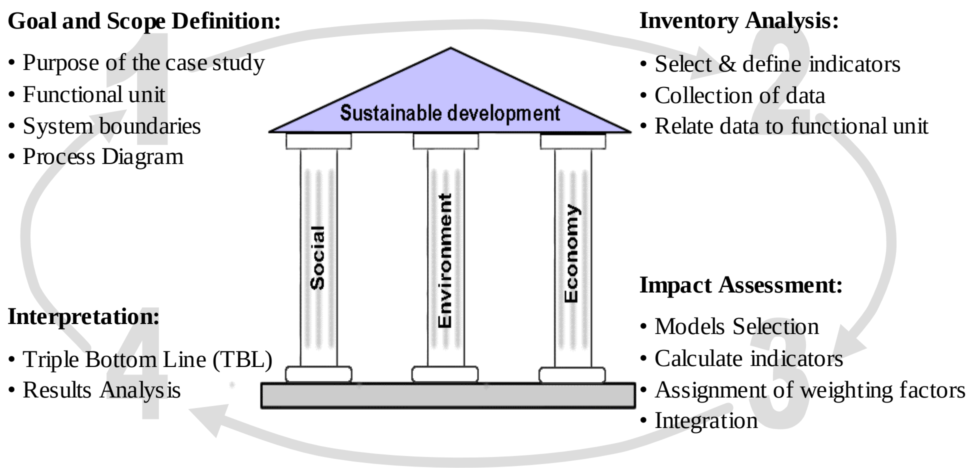

Figure 9. Integration of ISO 14040 framework within the three pillars of sustainability.

3.1. Functional Unit

The methodology proposed was made thinking in a product approach. All life cycle stages will be analyzed thinking in the impacts that the product can produce in the economy, society and environment. Consequently, the functional unit will be the produced unit (numbers of produced units or kg of production).

3.2. The System Boundaries

The methodology was conceived inside the framework of the existent interrelation between the production processes and the three pillars of sustainability, where each production process is a process chain that has its own inputs and outputs. The new methodology allows analyzing and comparing each stage of the life cycle of the production processes separately or as a whole. If the lifecycle is analyzed as a whole, there will be taking into account only one group of inputs: capital, labour, energy and raw materials; and one group of outputs: the products and wastes & emissions, as in Figure 10. If the life cycle is analyzed separately or by process unit, the products of each stage are going to be the raw materials for the next one Figure 11.

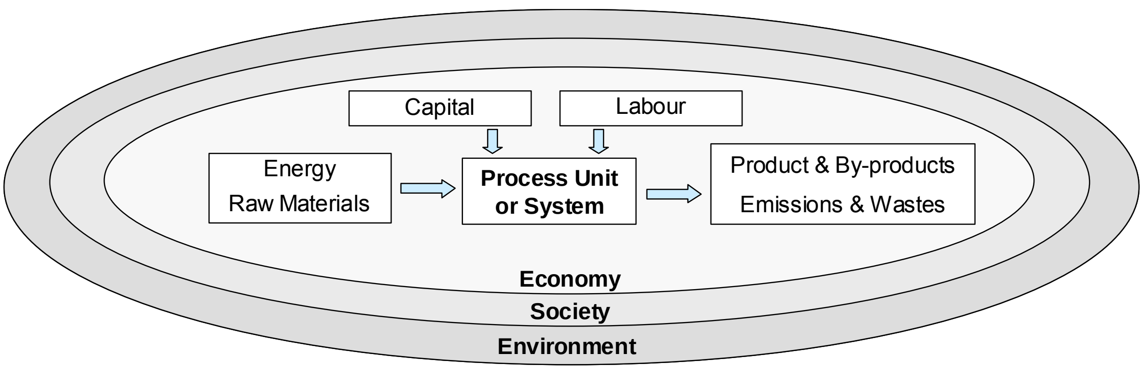

Figure 10. Inputs and outputs of a life cycle analysis performed as a whole.

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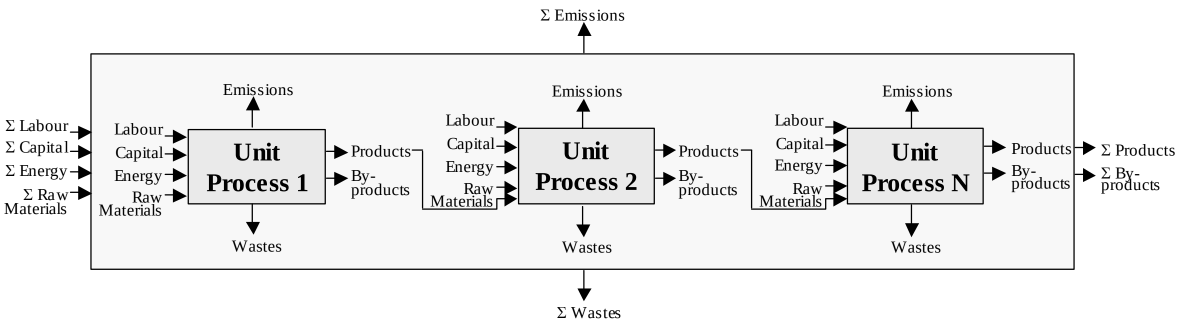

Figure 11. Inputs and outputs of a life cycle analysis performed by process unit.

The boundaries of the production process will depend on the goal and scope of the study, but each stage of the life cycle of the product has to be well defined. The boundaries are case-specific due to different products can have different effects in the scenario analyzed, that can be global, regional or local. Also different time horizon can be analyzed.

Each stage produces impacts that will be measured with indicators, in order to facilitate the developed tool. A general analysis is presented in the next section.

4. Inventory Analysis

In this step, impact categories, calculation methods, flows to be taken into account in the calculation must be selected, and the data collection must be done in order to obtain the correspondent inventory for each technology to be compared.

4.1. Indicators Selection

Adding the second, third and four requirements of the methodology described above, it was established that the SLCM methodology must allows the analysis of the impacts associated to the product in the three areas of sustainability through all stages of the life cycle of the product analyzed by using a small set of few lead indicators of each area, including a procedure to select this indicators and the results must be shown separately.

According to (Afgan and Carvalho, 2004), the effective indicator has to meet characteristics reflecting a problem and criteria to be considered. It must show how well a system is working. In case there is a problem, an indicator has to indicate its origin and the direction to be taken in order to solve the problem. The indicators have to meet certain specific requirements, as: to be relevant, understandable, and reliable (Liposcak et al., 2006). Commonly accepted indicator selection criteria can be found in the literature (Adriaanse, 1993; OECD, 1993; McLaren, 1996; Hardi and Zdan, 1997; Bossel, 1999; Lopez-Ridaura et al., 2002; Lamberton, 2005) and state that a good sustainability indicator should be:

- scientifically valid, meaning that there is an international consensus about its validity,
- representative of a broad range of conditions,

- responsive to changes in the environment and relevant to the needs of potential users,
- based on accurate and accessible data, that are available over time,
- understandable by potential users, comparable with indicators developed in other jurisdictions. Indicator should have a threshold or reference value against which to be compared, so that users are able to assess the significance of the values associated with it.
- cost-effective to collect and use, and unambiguous,
- limited in number, simple, and easy to interpret but, in aggregate, they should be comprehensive in their coverage of the goals of sustainable development,
- flexible enough to incorporate new scientific information and changing public perception.

The criteria mentioned above are general and describe the "ideal" indicator; not all of them will be met in practice (OECD, 1993). Each company or community will choose the indicators according to its specific purposes and trying to meet the most of the criteria mentioned above.

There is a wide gamma of indicators. The problem is not lack of indicators, but selects the right ones. The selection of the indicators for the three areas must be done taking into account the existent trade-off between sustainability areas. Also, different procedures to select indicators can be used for each area. In addition, each project is different; so, the selection of the indicators can be assumed as case-specific. It is important to note that all existent indicators can be calculated with the required data by their own methods, but to obtain the sustainability index, a small set of few significant indicators will be used to analyze the impacts of each area (Kemmler and Spreng, 2007), and these indicators must be well selected in order to obtain a representative analysis (Azapagic, 2004).

As the SLCM methodology must be based on ISO 14040 series for environmental LCA, and knowing that LCT philosophy have been applied to the environmental field as LCA, to the economic area as LCC, and in the social area few works have been published (see Chapter 1 section 1.3); it is recommended to use LCA indicators for environmental assessment, LCC indicators for economical evaluation, Social Life Cycle (SLC) indicators for social analysis within SLCM methodology. A short analysis of selection of indicators is explained below.

It is also important to note that in this work a procedure to select the indicators have been developed, and some lead indicators are identified, but the methodology can be applied to any process or activity choosing in each case the corresponding set of inventory data and sustainability impact indicators. Even when some indicators are identified for each area, a sensitivity analysis is recommended in order to identify the indicators of each area that are more affected by changes in the inputs. The indicators identified in the sensitivity analysis will be the most recommended to be used in the sustainability analysis.

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Environmental area

An inventory of raw materials, energy, water, and emissions and wastes generated must be done. If experimental data is not available, this inventory can be obtained theoretically by using mass and energy balances and process simulations. With this inventory several environmental indicators can be calculated.

It is recommended to calculate the environmental impacts using LCA. But, there are diverse indicators that can be used for this calculation. Even when the CML 2001 baseline methodology will be used in this work, an indicators' selection must be done between the ones presented by this methodology. Therefore, a procedure to select environmental LCA indicators was developed taking as inspiration some previous works (Udo de Haes et al., 1999a, 1999b; Herrera Orozco, 2004).

First, for the development of this indicators selection procedure an analysis of common processes inputs and output was made. A common process use raw materials that can be water, energy and/or resources as inputs, and produces products, by-products, emissions and wastes, as it is shown in Figure 12.

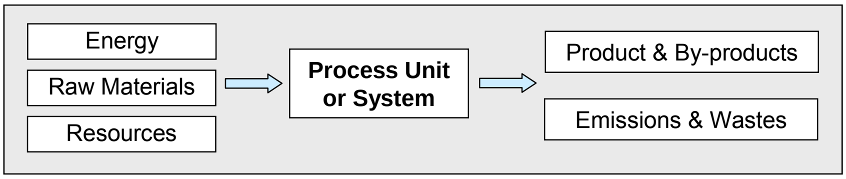

Figure 12. Common process inputs and outputs

From the environmental point of view it is important to analyze the consumption of these inputs and the emissions and wastes produced. Therefore, as a second step, an analysis of the inputs has to be done in order to determine what kinds of inputs are used in the process and in what quantity these inputs are consumed. Knowing the inputs, the related impact indicators must be calculated. In order to facilitate the developed tool an indicators selection procedure based on process inputs was developed, as it is shown in Figure 13. Even when resources can be living and non-living, in this procedure only non-living resources were taken into account, based on the assumption that the process that are going to be analyzed do not use living resources. If living resources are going to be used in the process to analyzed, the impact category "Depletion of biotic resources" must be included in the indicators selection procedure.

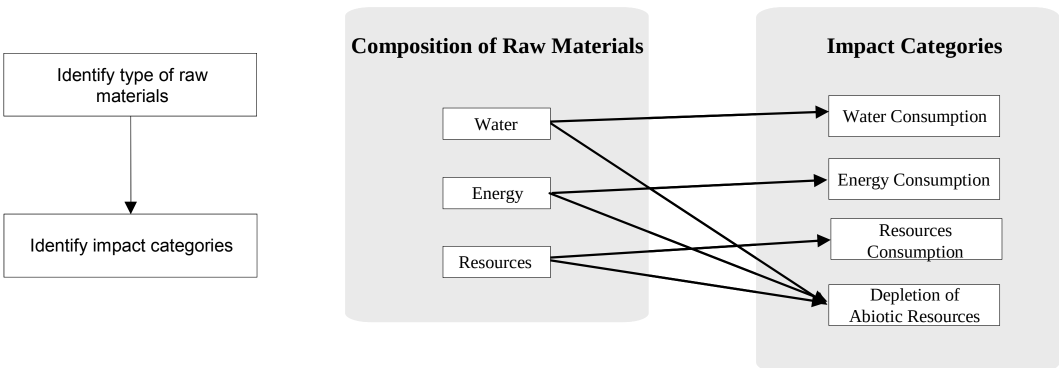

Figure 13. Environmental indicators selection procedure based on process inputs

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As a third step, as in the case of the inputs, an analysis of the outputs has to be done in order to determine what kinds of outputs are produced in the process and in what quantity. Once the outputs produced are known, the related impact indicators must be calculated. In order to facilitate the use of the developed tool an indicators selection procedure based on process outputs was developed, as it is shown in Figure 14.

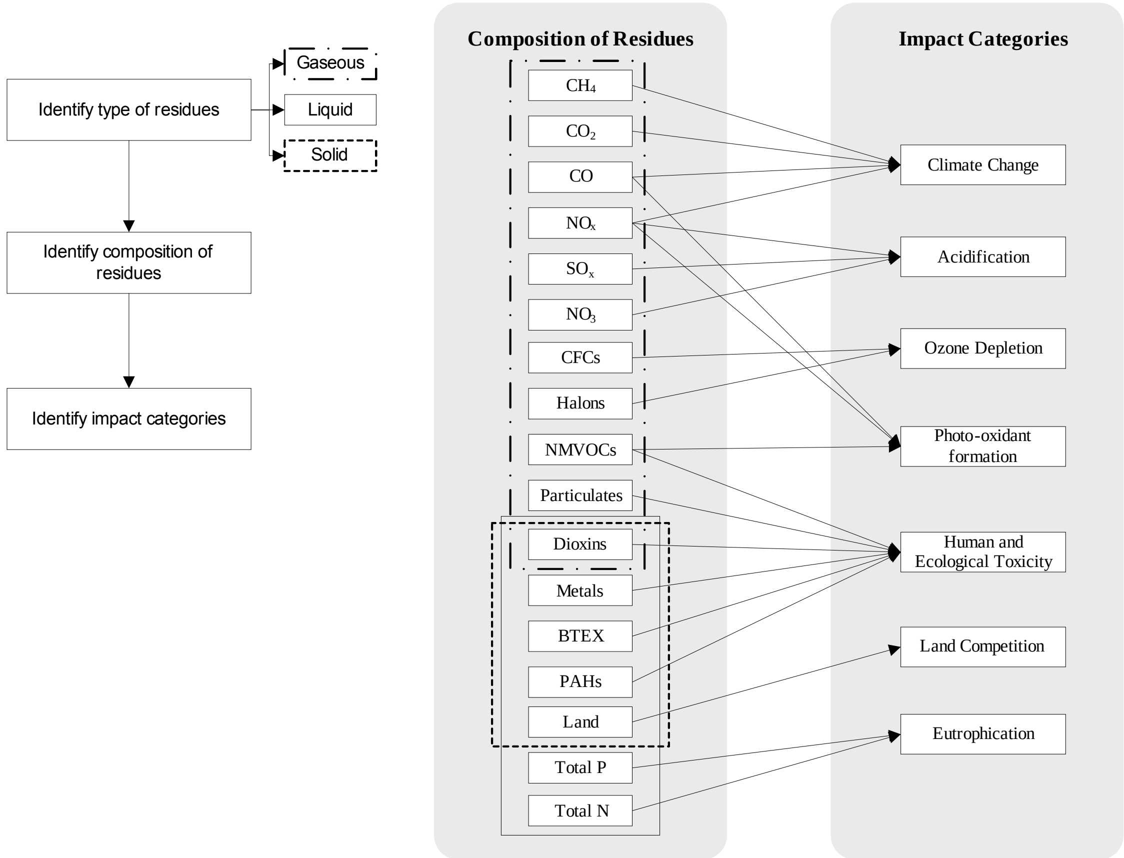

Figure 14. Environmental indicators selection procedure based on process outputs

Some of the indicators mentioned above can be used to assess the environmental area and can also be used to express environmental eco-efficiency, as: consumption of raw materials, energy, and water, and emissions and wastes generated.

Two groups of indicators are proposed for environmental assessment: LCA indicators, and environmental eco-efficiency indicators. Indicators of each group or a complete group can be selected for environmental evaluation. The indicators proposed are shown in Table 10.

Table 10. Indicators proposed for environmental assessment.

LCA indicators	Eco-Efficiency indicators
Depletion of abiotic resources	Consumption of raw materials
Climate change	Consumption of energy
Acidification	Consumption of water
Stratospheric ozone depletion	Emissions and wastes generated
Photo-oxidant formation	
Human and Ecological toxicity	
Land competition	
Eutrophication	

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With the composition of the raw materials and the composition of the residues, some environmental indicators can be easily selected and a list of few (from 3 to 6) lead indicators can be obtained. Then, with the help of the goal and scope of the project to be study this list can be improved in order to obtain a more refined list. It is important to note that always the indicators selection procedure will depend on the goal and scope of the project.

Use of Proxies

When dealing with new processes, probably part of the data will not be available. In case that the flow of an input/output streams is not known, we should estimate its value based on mass balances, experience, etc. In case that information about the nature of the substance or the substance is not available in the environmental database, a proxy should be considered instead. This proxy is selected from a list of products with similar physical and/or chemical properties.

To assure the validity of the proxy approach it is convenient to run a sensitivity analysis to check the effect of the proxy variable on the sustainable indicators. If this effect can be reflected, the effect of the variable can be discarding. In a contrary case a more reliable data should be used in the calculations.

Economic area

Usually, industries use indicators as VPN, TIR, IRR, PP, etc. (see Chapter 2, section 3) to evaluate their projects, and these are good indicators to do so. To use these indicators a period of time must be defined and the result is a value that represents the performance of the process unit or system for the complete period of time defined. But, in this methodology, the functional unit is a produced unit which is a small part of the project and not a period of time. Thus, if a period of time is defined, it cannot be assured that just one functional unit is going to be produced, i.e. if the period of time is defined as 1 year and the functional unit is 1 kg of produced product; in 1 year maybe a thousands of functional units can be produced. Therefore, to use these indicators in this methodology, a period of time have to be defined at the beginning, and after the calculations, the result, have to be transformed into the functional unit selected to know the economical impact of the functional unit.

Maybe, it can be easy to calculate monetary flows that occur during the life of a product, from the initial cost to the product's disposal, as in life cycle costing. In this case, the indicators can be: the complete LCC or capital cost/initial investment, operation and maintenance cost, energy cost, water cost, external costs, etc., and these costs will be related to the functional unit. Some of these indicators can also be used to express economical eco-efficiency.

Three groups of indicators are proposed for economical assessment: general indicators, LCC indicators, and eco-efficiency indicators. Indicators of each group or a complete group can be selected for economical evaluation. The indicators proposed are shown in Table 11.

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Table 11. Indicators proposed for economical assessment.

General indicators	LCC indicators	Eco-Efficiency indicators
VPN	Capital cost/initial investment	Raw materials cost
TIR	Operation and maintenance cost	Energy cost
IRR	Energy cost	Water cost
PP	Water cost	Residues treatment cost
LCC	External costs	

Since each proposed economical indicators group, covers the complete economical aspect of a project, it is recommended to select a complete group of indicators in order to obtain a list of few (from 3 to 6) lead indicators. Then, with the help of the goal and scope of the project to be studied, this list can be complemented with indicators from another group in order to obtain a more refined list. Please note that eco-efficiency and LCC indicators are related, and LCC indicators include eco-efficiency ones. Therefore, it is not recommended to select LCC indicators group and complement with indicators from eco-efficiency group or vice versa. Instead, it is recommended to select LCC or eco-efficiency indicators group and complement the list with indicators from general group or vice versa. It is important to note that always the indicators selection procedure will depend on the goal and scope of the project.

Social area

As there are so few works on SLCA, a short analysis of the situation will be done first in order to propose some indicators.

As it was shown in Chapter 2 section 4, SLCA methodologies mainly include the worker and the society. Related with the worker, the methodologies make a distinction between the worker situation and the health & safety in the working place. Related with society, the methodologies try to evaluated equity as mean of gender and race.

Therefore, these four groups (worker situation, health & safety, gender, and diversity) will be analyzed in the SLCM methodology by some proposed indicators. Indicators of each group or a complete group can be selected for social evaluation. The indicators proposed are shown in Table 12.

Table 12. Indicators proposed for social assessment.

Worker situation	Health & Safety	Gender equity	Diversity equity
• Remuneration • Promotion rate • Training and education • Ratio between fixed and temporal employees, in number and remuneration	• Lethal accidents • Non-lethal accidents • Heaviness of work • Inherent safety index • Hazard Identification and Ranking (HIRA)	• Equal number of men and women • Equal remuneration for men and women • Share of women work	• Equal number of local and foreign employees • Equal remuneration for local and foreign employees

From the four proposed social indicators groups, each one analyzes a different area of the social aspect. Each of these areas is important to obtain a complete analysis of the social part (Chapter 2 section 4). Therefore, it is recommended to select at least one indicator of each group in order to obtain a list of few (from 3 to 6) lead indicators. This

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list will be refined and complemented with other indicators, according to the goal and scope of the project under study. It is important to note that always the indicators selection procedure will depend on the goal and scope of the project.

5. Life Cycle Impact Assessment

In this step, the impacts have to be calculated, and the principal flows contributing to these impacts have to be identified. The calculation method must be equal to all the technologies to be compared, but the calculation and results must be presented separately. Then, weighting factors must be assign to these indicators based on AHP in order to integrate the three pillars of sustainability into one overall sustainability index.

As it was explained in Chapter 2 section 2.1 and Chapter 3 section 4.1, all existent indicators can be calculated by their own method, but to obtain the sustainability index is useful to use a small set of few lead indicators that have to be aggregated in an overall sustainability index. For this aggregation it is recommended to use a minimum of three (3) indicators and a maximum of six (6) indicators of each area, because less than 3 indicators will not produce a realistic result and more than 6 indicators will produce difficult to interpret results. If a wide gamma of indicators is required to analyze a specific project, the use of fuzzy logic is proposed for this type of analysis (Andriantiatsaholiniaina et al., 2004). Some indicators were proposed in Chapter 3 section 4.1, and in this section the procedure to aggregate the indicators will be explained.

5.1. Indicators Aggregation

The integration part of the methodology will consist on five steps: 1) indicators prioritization and normalization, to prioritize and normalize the indicators results, 2) weighting per indicators, to assign preferences to the indicators in each group, 3) weighting per groups, to assign preferences to the groups, 4) weighting prioritization, to obtain the global weighting value of each indicator, 5) sustainability ranking, to obtain the overall sustainability index.

In this section, a general description of the indicators aggregation is given. In Chapter 4 and Chapter 5, the calculation procedure is shown in detail.

1) Indicators prioritization and normalization
A pair wise comparison per indicator based on the analytical hierarchical process (Ong et al., 2001) must be done. This procedure has to be done for each indicator to obtain the prioritization and normalization per indicators. Figure 15 shows the pair wise comparison per indicators procedure.

In this figure, several scenarios (j: 1, 2, .., n) are compared by means of several indicators (i: 1, 2, ..., n). The value of each indicator in the scenarios compared is represented as A_{ij} for the first indicator, B_{ij} for the second, and consequently.

Then a matrix is built for each one of the indicators, where D ij values in the matrix are obtained as follows:

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If i = j, then $D_{ij} = 1$
If i < j, then $D_{ij} = A_{ii}/A_{ij}$
If i > j, then $D_{ij} = 1/D_{ji}$
Sumatory values (Σi) are obtained for each scenario, and are then used to normalize the calculated D_{ij} ratios, thus obtaining the normalised values (E_{ij}). An average (Fij) of the normalised values is finally obtained for each scenario and indicator.

2) Weighting per indicators
The indicators selected must be weighted. The assignment of the weighting factors (G_{ij}) is based on expert judge and bibliography. The weighting procedure is based on a pair wise comparison between indicators per groups (environment, social, economic). This means that the indicators (i: 1, 2, ..., n) of each group must be compared with the other indicators (j: 1, 2, ..., n) of the same group. It is assumed that indicators with different units are not comparable. Figure 16 shows the weighting per indicators procedure.

In this figure, the G_{ij} values are the weighting factors assigned by the user to each of the indicators. G_{ij} values are agregated (Σi) and normalized (H_{ij}). The average of the normalized values (I_{ij}) is obtained as the indicators weighting list, for each of the indicators in a group.

It is important to note that the indicators weights can vary according to the case study.

	$Scenario_1$	$Scenarior_2$	$Scenario_n$
$Indicator_1$	A_{11}	A_{12}	A_{1n}
$Indicator_2$	B_{21}	B_{22}	B_{2n}
$Indicator_n$	C_{n1}	C_{n2}	C_{nn}

	$Scenario_1$	$Scenarior_2$	$Scenario_n$
$Indicator_1$	A_{11}	A_{12}	A_{1n}

	$Scenario_1$	$Scenario_2$	$Scenario_n$
$Scenario_1$	$D_{11}=A_{11}/A_{11}$	$D_{12}=A_{11}/A_{12}$	$D_{1n}=A_{11}/A_{1n}$
$Scenario_2$	$D_{21}=1/W_{12}$	$D_{22}=A_{12}/A_{12}$	$D_{2n}=A_{12}/A_{1n}$
$Scenario_n$	$D_{n1}=1/W_{13}$	$D_{n2}=1/W_{23}$	$D_{nn}=A_{1n}/A_{1n}$
	$\Sigma1=D_{11}+D_{21}+D_{n1}$	$\Sigma2=D_{12}+D_{22}+D_{n2}$	$\Sigma n=D_{1n}+D_{2n}+D_{nn}$

	$Scenario_1$	$Scenario_2$	$Scenario_n$
$Scenario_1$	$E_{11}=D_{11}/\Sigma1$	$E_{12}=D_{12}/\Sigma2$	$E_{1n}=D_{1n}/\Sigma n$
$Scenario_2$	$E_{21}=D_{21}/\Sigma1$	$E_{22}=D_{22}/\Sigma2$	$E_{2n}=D_{2n}/\Sigma n$
$Scenario_n$	$E_{n1}=D_{n1}/\Sigma1$	$E_{n2}=D_{n2}/\Sigma2$	$E_{nn}=D_{nn}/\Sigma n$

	Average for $Indicator_1$
$Scenario_1$	$F_{11}=(E_{11}+E_{12}+E_{1n})/n$
$Scenario_2$	$F_{21}=(E_{12}+E_{22}+E_{2n})/n$
$Scenario_n$	$F_{n1}=(E_{n1}+E_{n2}+E_{nn})/n$

	Group 1 to n		
	$Indicator_1$	$Indicator_2$	$Indicator_n$
$Scenario_1$	F_{11}	F_{12}	F_{1n}
$Scenario_2$	F_{21}	F_{22}	F_{2n}
$Scenario_n$	F_{n1}	F_{n2}	F_{nn}

Figure 15. Indicators prioritization and normalization scheme

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	$Indicator_1$	$Indicator_2$	$Indicator_n$
$Indicator_1$	G_{11}	G_{12}	G_{1n}
$Indicator_2$	G_{21}	G_{22}	G_{2n}
$Indicator_n$	G_{n1}	G_{n2}	G_{nn}
	$\Sigma1=G_{11}+G_{21}+G_{n1}$	$\Sigma2=G_{12}+G_{22}+G_{n2}$	$\Sigma n=G_{1n}+G_{2n}+G_{nn}$

	$Indicator_1$	$Indicator_2$	$Indicator_n$
$Indicator_1$	$H_{11}=G_{11} / \Sigma1$	$H_{12}=G_{12} / \Sigma2$	$H_{1n}=G_{1n} / \Sigma n$
$Indicator_2$	$H_{21}=G_{21} / \Sigma1$	$H_{22}=G_{22} / \Sigma2$	$H_{2n}=G_{2n} / \Sigma n$
$Indicator_n$	$H_{n1}=G_{n1} / \Sigma1$	$H_{n2}=G_{n2} / \Sigma2$	$H_{nn}=G_{nn} / \Sigma n$

	Average per Indicator
$Indicator_1$	$I_{11}=(H_{11}+H_{12}+H_{1n})/n$
$Indicator_2$	$I_{21}=(H_{12}+H_{22}+H_{2n})/n$
$Indicator_n$	$I_{n1}=(H_{n1}+H_{n2}+H_{nn})/n$

	Weighting per Indicator
$Indicator_1$	I_{11}
$Indicator_2$	I_{21}
$Indicator_n$	I_{n1}

Figure 16. Weighting per indicator scheme

3) Weighting per groups
The groups to be analyzed (environment, social, economic) must be weighted. The assignment of the weighting factors is based on expert judge and bibliography. The weighting procedure is based on a pair wise comparison between groups. It is assumed that different groups are not comparable. Figure 17 shows the weighting per group procedure.

In this figure, the J_{ij} values are the weighting factors assigned by the user to each of the groups. As in the weighting per indicators case, the assignement of weighting factors is is based on expert judge and bibliography. J_{ij} values are agregated (Σi) and normalized (K_{ij}). The average of the normalized values (L_{ij}) is obtained as the indicators weighting list, for each of the groups.

It is important to note that the group's weights can vary according to the case study.

4) Weighting prioritization
The weight per indicator (I_{ij}) has to be multiplied per the weight per group (L_{ij}) to obtain the global weighting prioritization (M_{ij}). After the calculations, the weighting prioritization is obtained. Figure 18 shows the weighting prioritization scheme.

5) Sustainability Ranking
The sustainability ranking of the indicators is obtained by multiplying the indicators prioritization (F_{ij}, in Figure 15) per the weighting prioritization (M_{ij}, in Figure 18) of each technology. These products (N_{ij}) are agregated to obtain the sustainability ranking values (R_{ij}). Figure 19 shows the sustainability ranking scheme.

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	Group$_1$	Group$_2$	Group$_n$
Group$_1$	J_{11}	J_{12}	J_{1n}
Group$_2$	J_{21}	J_{22}	J_{2n}
Group$_n$	J_{n1}	J_{n2}	J_{nn}
	$\Sigma 1=J_{11}+J_{21}+J_{n1}$	$\Sigma 2=J_{12}+J_{22}+J_{n2}$	$\Sigma n=J_{1n}+J_{2n}+J_{nn}$

	Group$_1$	Group$_2$	Group$_n$
Group$_1$	$K_{11}=J_{11} / \Sigma 1$	$K_{12}=J_{12} / \Sigma 2$	$K_{1n}=J_{1n} / \Sigma n$
Group$_2$	$K_{21}=J_{21} / \Sigma 1$	$K_{22}=J_{22} / \Sigma 2$	$K_{2n}=J_{2n} / \Sigma n$
Group$_n$	$K_{n1}=J_{n1} / \Sigma 1$	$K_{n2}=J_{n2} / \Sigma 2$	$K_{nn}=J_{nn} / \Sigma n$

	Average per Group
Group$_1$	$L_{11}=(K_{11}+K_{12}+K_{1n})/n$
Group$_2$	$L_{21}=(K_{12}+K_{22}+K_{2n})/n$
Group$_n$	$L_{n1}=(K_{n1}+K_{n2}+K_{nn})/n$

	Weighting per Group
Group$_1$	L_{11}
Group$_2$	L_{21}
Group$_n$	L_{n1}

Figure 17. Weighting per group scheme

		Weighting Prioritization
Group$_1$	Indicator$_1$	$M_{11}=I_{11}*L_{11}$
	Indicator$_2$	$M_{21}=I_{21}*L_{11}$
	Indicator$_n$	$M_{n1}=I_{n1}*L_{11}$
Group$_n$	...	...

Figure 18. Weighting prioritization scheme

	Group$_1$			…	Sustainability Ranking
	Indicator$_1$	Indicator$_2$	Indicator$_n$	…	
Scenario$_1$	$N_{11}= F_{11} * M_{11}$	$N_{12}= F_{12} * M_{21}$	$N_{1n}= F_{1n} * M_{n1}$	…	$R_{11}=N_{11}+N_{12}+N_{1n}$
Scenario$_2$	$N_{21}= F_{21} * M_{11}$	$N_{22}= F_{22} * M_{21}$	$N_{2n}= F_{2n} * M_{n1}$	…	$R_{21}=N_{21}+N_{22}+N_{2n}$
Scenario$_n$	$N_{n1}= F_{n1} * M_{11}$	$N_{n2}= F_{n2} * M_{21}$	$N_{nn}= F_{nn} * M_{n1}$	…	$R_{n1}=N_{n1}+N_{n2}+N_{nn}$

	Sustainability Ranking
Scenario$_1$	R_{11}
Scenario$_2$	R_{21}
Scenario$_n$	R_{n1}

Figure 19. Sustainability ranking scheme

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6. Interpretation

In order to accomplish requirements sixth and seventh of the methodology, in this step, an identification of the most important results and an evaluation of the study's outcomes (sensitivity and uncertainty analysis) must be done, followed by the presentation of results in a triple bottom line framework, in order to identify the strengths and weaknesses points of each technology and the responses to the defined objective. In addition a comparison of the results obtained for each technology analyzed must be drawn and conclusions, recommendations and reports must be written.

6.1. Sensitivity and Uncertainty Analysis

To calculate indicators and sustainability index, mathematical models are used based on series of equations, input factors, parameters, and variables aimed to characterize the process being investigated. These bases are subject to many sources of uncertainty including errors of measurement, absence of information, use of proxies, and poor or partial understanding of the driving forces and mechanisms. Therefore, each of these bases must be analyze in order to identify possible sources of uncertainty and variability.

In SLCM methodology the environmental, economical and social area are analyzed by impact indicators and aggregate by assigning weighting to the impacts selected. Each area uses a different mathematical model to calculate their indicators. For the calculation, each mathematical model requires general information about the process and specific data related to the indicators of each area. Also, the selection of indicators and the assignment of weighing factors have an associated uncertainty that must be taken into account. A detailed analysis of the general and specific data required for the uncertainty calculation is done below, and to analyze these uncertainties, with SLCM methodology, a sampling model (Monte Carlo) can be used. Even when the sensivity and uncertainty analysis is explained in detailed, it was not applied to the case studies.

Environmental area

In order to calculate the environmental impacts, the following general equation is used:

$$EI = Inventory \times EV \times CF$$

where *EI* is the environmental impact calculated (i.e. global warming potential), *Inventory* is the data of all inputs and outputs related with the process (see Chapter 2 section 2.1 Life Cycle Inventory Analysis), *EV* is the eco-vector or environmental vector which is the set of environmental burdens identified in a life cycle inventory that can be associated with an input or output flow or with the life cycle of an equipment unit and this data can be found in databases (i.e. Ecoinvent), *CF* is the characterization factor associated to each environmental impact that can be found in databases (i.e. Ecoinvent).

In this equation, uncertainty can arise from different sources:

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- Inventory. The inventory can be a constant value (i.e. when a quantity of raw material cannot be changed by the formulation or the process) or the inventory can vary (i.e. when a quantity of raw material can be changed between a range specified by the formulation or the process). In this study the uncertainty of the inventory will depend on the formulation or process to be study and can be taken into account.
- Eco-Vector. In this study, the eco-vectors have an uncertainty associated in databases that can be taken into account.
- Characterization factors. In databases, characterization factors do not have an associated uncertainty. Even when it is known that characterization factor are calculated for a specific scenario and that it can vary depending on the case analyzed, in this study the characterization factors will be considered as constants.

Economic area

In order to calculate the economic impacts, the following general equation is used:

$$EcI = Inventory \times Cost$$

where *EcI* is the economical impact calculated (i.e. cost of raw materials used in the process), *Inventory* is the data of all inputs and outputs related with the process (see Chapter 2 section 2.1 Life Cycle Inventory Analysis), *Cost* is the economical cost associated to each economical impact that can be found in the market (i.e. cost of steam).

In this equation, uncertainty can arise from different sources:

- Inventory. As in the environmental area, the inventory can be a constant value (i.e. when a quantity of raw material cannot be changed by the formulation or the process) or the inventory can vary (i.e. when a quantity of raw material can be changed between a range specified by the formulation or the process). In this study the uncertainty of the inventory will depend on the formulation or process to be study and can be analyzed.
- Cost. The costs can vary depending on the inflation rate, the supplier, the market, or the geographical region analyzed. In this study these variations of the cost can be considered.

Social area

In order to calculate the social impacts, the following two different equations are used:

$$SI = Inventory \times Characteristic \quad (1)$$

$$SI = f(Invenrory) \quad (2)$$

where *SI* is the social impact calculated (i.e. for (1): Inherent safety index; for (2): number of employees), *Inventory* is the data of all inputs and outputs related with the process (see Chapter 2 section 2.1 Life Cycle Inventory Analysis), *Characteristic* is referred to chemicals and process characteristics (i.e. chemicals: flammability; process: maximum temperature).

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In this equation, uncertainty can arise from different sources:

- Inventory. As in the environmental area, the inventory can be a constant value (i.e. when a quantity of raw material cannot be changed by the formulation or the process) or the inventory can vary (i.e. when a quantity of raw material can be changed between a range specified by the formulation or the process). In this study the uncertainty of the inventory will depend on the formulation or process to be study and can be taken into account.
- Characteristic. Some characteristics can vary (i.e. a process maximum temperature) and other characteristics cannot (i.e. a chemical flammability). In this study these variations of the cost can be considered.

Selection of indicators

Every selection between options procedure includes an uncertainty inherent to the selection procedure (i.e. why an option is selected instead of other one). Even when an indicators selection procedure was developed in this methodology, different indicators can be selected depending on the goal and scope of the project and this selection includes uncertainty. In this study the uncertainty of the indicators selection procedure will depend on the goal and scope of the project and can be taken into account.

Assignment of weighting factors

As in a selection procedure, every assignment of weighting procedure includes an uncertainty inherent to the assignment of weighting factors (i.e. why a weight is given to an option and different weight is given to other one). The assignment of weighting factors procedure, in this study, will depend on literature and will be justified, but different weights can be given to different indicators depending on the goal and scope of the project and this assignment of weighting include uncertainty. In this study the uncertainty of the indicators assignment of weighting procedure will depend on the goal and scope of the project and can be taken into account.

6.2. Communication of Results

The values obtained in the sustainability ranking step are plotted in a spider diagram in order to obtain a clearer visualization of the results. Figure 20 shows the results represented in a TBL framework.

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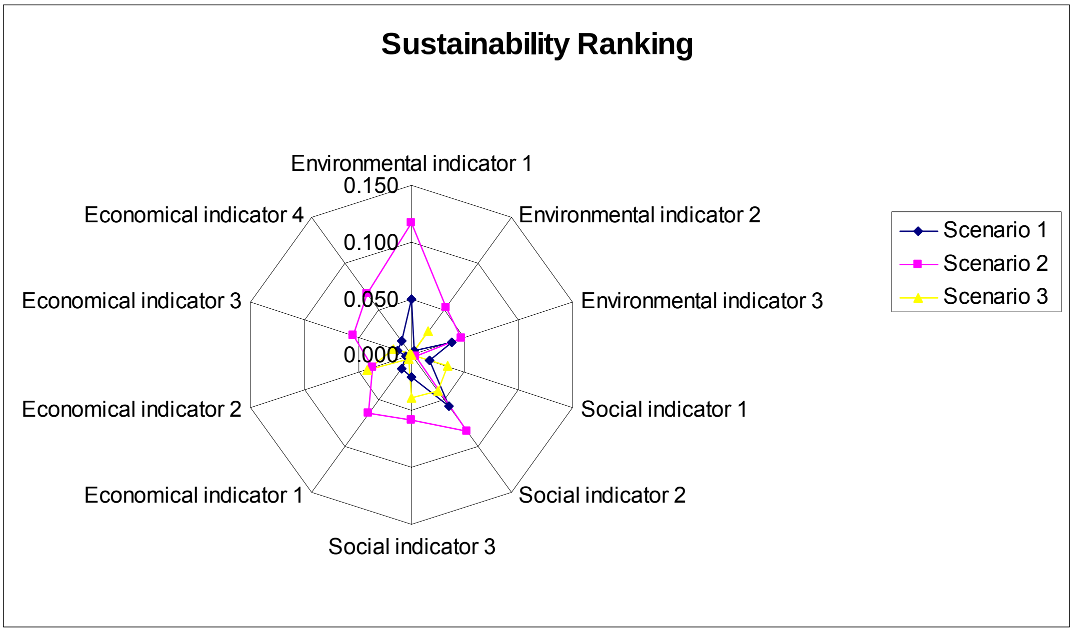

Figure 20. Triple bottom line framework

7. General Diagram of the SLCM Methodology

Based on the mentioned requirements and all explained steps, a general diagram of the SLCM methodology was developed. Figure 21 shows the SLCM methodology diagram, which follows all steps of the ISO 14040 series, showing the results of the indicators separately, with the innovation of the integration of the three pillars of sustainability where a normalization and weighting procedure based on the analytical hierarchical process takes place. The methodology includes a procedure for the selection of the indicators to be used in the sustainability index calculation. The results of the sustainability index are represented in a triple bottom line framework which allows seeing the weak points of each technique to compare and improve them if it is appropriate. Additionally, sensitivity and uncertainty analysis are performed to the results.

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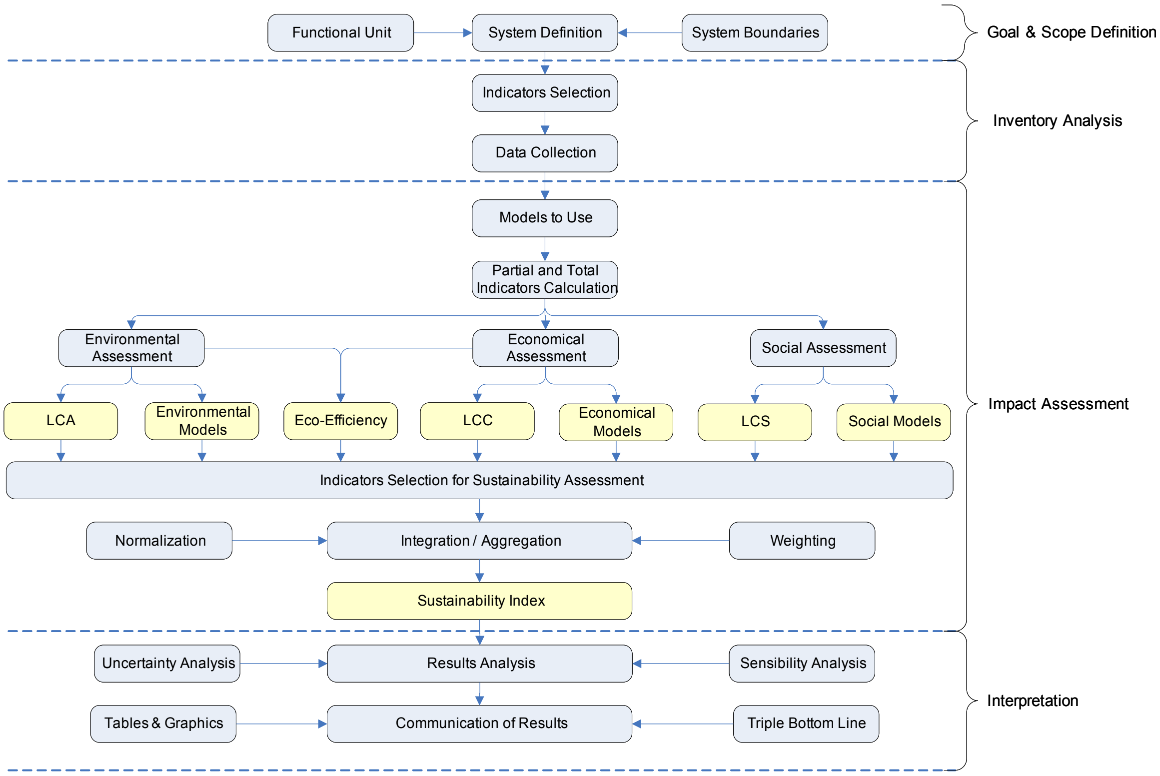

Figure 21. General diagram of the SLCM methodology

8. Calculation Procedure

The second objective of this research was to implement the SLCM methodology in a software application to assess processes with the possibility of comparing different production scenarios. To accomplish this objective, the SLCM methodology was: 1) translated to Microsoft® Excel® format, followed by 2) a Matlab© programming in order to obtain the sustainability module for MICAP software.

8.1. Translation to Microsoft® Excel® format

In order to translate the SLCM methodology to Microsoft® Excel® format, the four steps of ISO 14040 standards was followed with the innovation of the integration of the three pillars of sustainability in each step: goal and scope definition, inventory analysis, impact assessment, and interpretation.

Goal and Scope Definition

In this step, a Microsoft® Excel® sheet was made to define the functional unit and set the system boundaries and assumptions for the environmental, economic and social aspects, for each technology analyzed and compared (see Figure 22).

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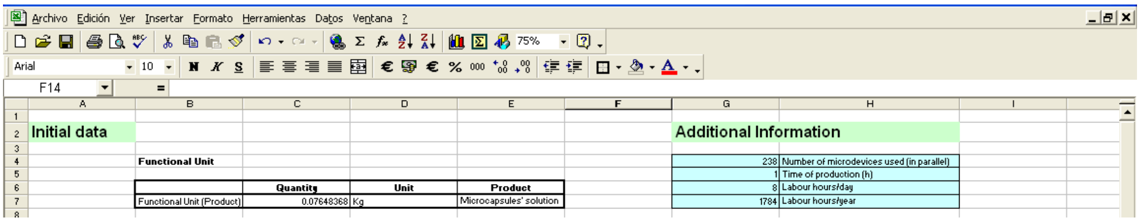


Initial data

Functional Unit

	Quantity	Unit	Product
Functional Unit (Product)	0.07648368	Kg	Microcapsules' solution

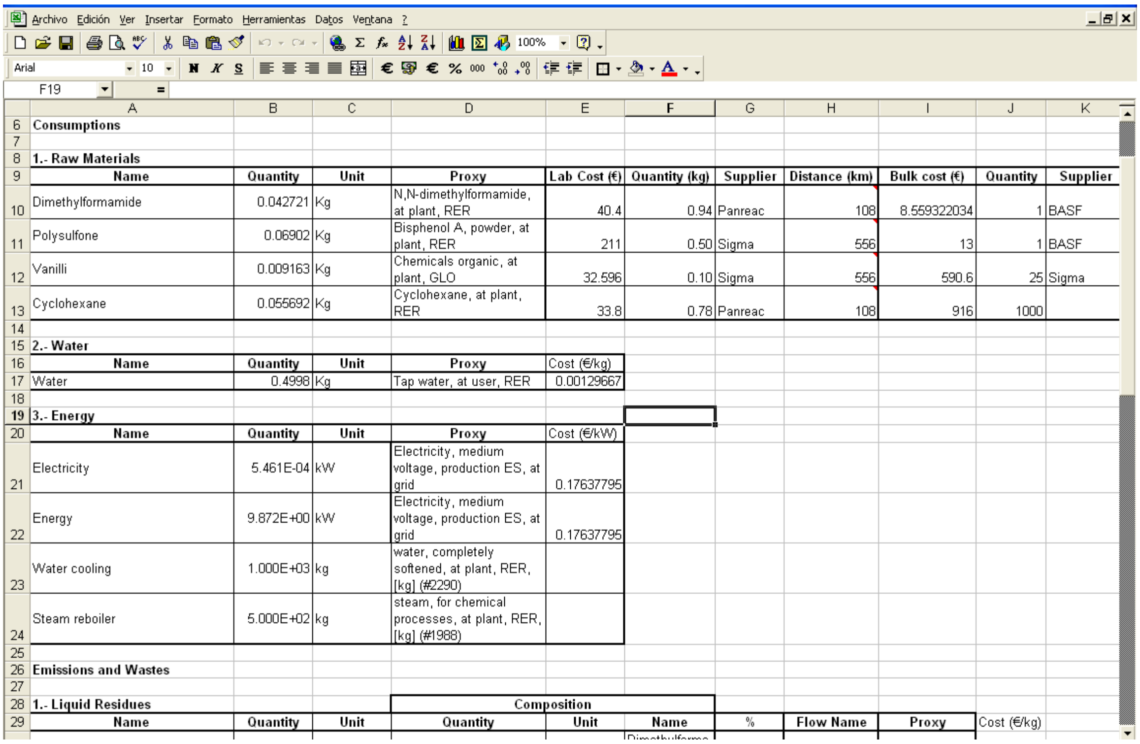
Additional Information

238	Number of microdevices used (in parallel)
1	Time of production (h)
8	Labour hours/day
1784	Labour hours/year

Figure 22. Goal and Scope Definition Data Sheet

Inventory Analysis

In this step, a Microsoft® Excel® sheet was made to collect all data for the environmental, economic and social impacts calculation, for each technology analyzed and compared (see Figure 23).



Consumptions

1.- Raw Materials

Name	Quantity	Unit	Proxy	Lab Cost (€)	Quantity (kg)	Supplier	Distance (km)	Bulk cost (€)	Quantity	Supplier
Dimethylformamide	0.042721	Kg	N,N-dimethylformamide, at plant, RER	40.4	0.94	Panreac	108	8.559322034	1	BASF
Polysulfone	0.06902	Kg	Bisphenol A, powder, at plant, RER	211	0.50	Sigma	556	13	1	BASF
Vanilli	0.009163	Kg	Chemicals organic, at plant, GLO	32.596	0.10	Sigma	556	590.6	25	Sigma
Cyclohexane	0.055692	Kg	Cyclohexane, at plant, RER	33.8	0.78	Panreac	108	916	1000	

2.- Water

Name	Quantity	Unit	Proxy	Cost (€/kg)
Water	0.4998	Kg	Tap water, at user, RER	0.00129667

3.- Energy

Name	Quantity	Unit	Proxy	Cost (€/kW)
Electricity	5.461E-04	kW	Electricity, medium voltage, production ES, at grid	0.17637795
Energy	9.872E+00	kW	Electricity, medium voltage, production ES, at grid	0.17637795
Water cooling	1.000E+03	kg	water, completely softened, at plant, RER, [kg] (#2290)	
Steam reboiler	5.000E+02	kg	steam, for chemical processes, at plant, RER, [kg] (#1988)	

Emissions and Wastes

1.- Liquid Residues

Name	Quantity	Unit	Composition: Quantity	Composition: Unit	Composition: Name	%	Flow Name	Proxy	Cost (€/kg)

Figure 23. Inventory Analysis Data Sheet

Life Cycle Impact Assessment

In this step, different Microsoft® Excel® sheets were made, for each technology analyzed and compared: 1) to calculate environmental, economic and social impacts (see Figure 24, Figure 25, and Figure 26), and 2) to integrate the three pillars of sustainability into one overall sustainability index (see Figure 27, Figure 28, and Figure 29).

To calculate the environmental impacts, eco-vectors data were taken from Ecoinvent database v2.0.

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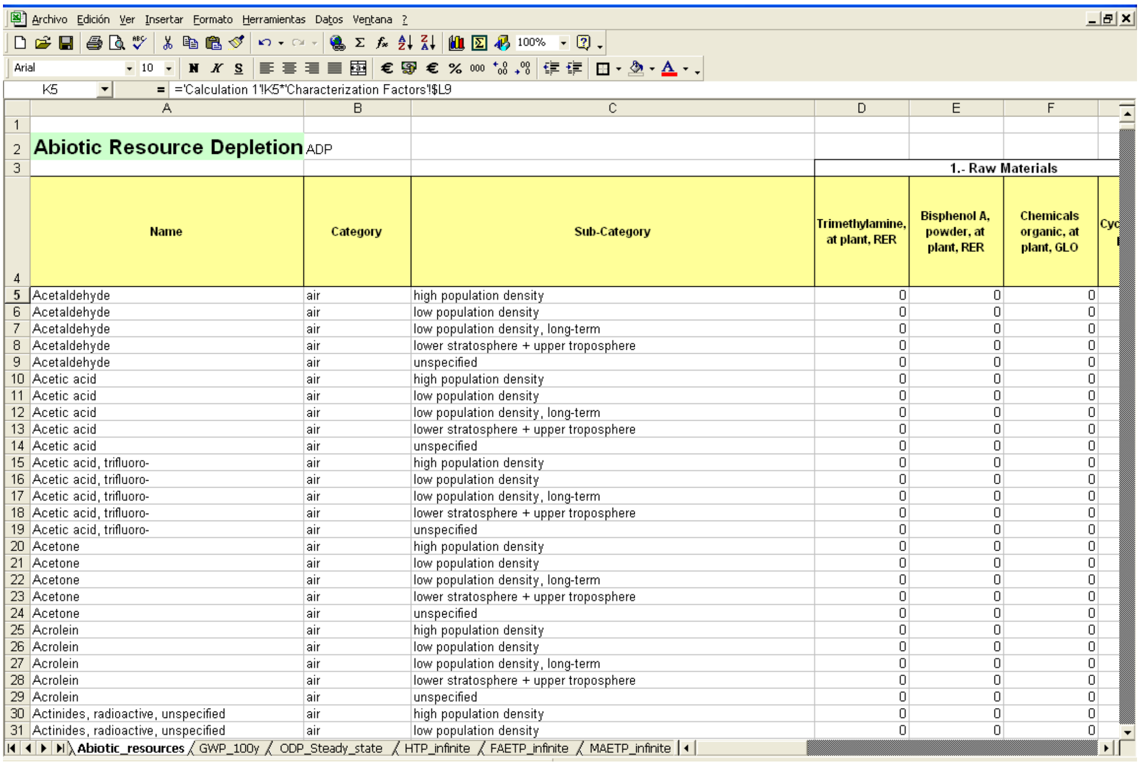
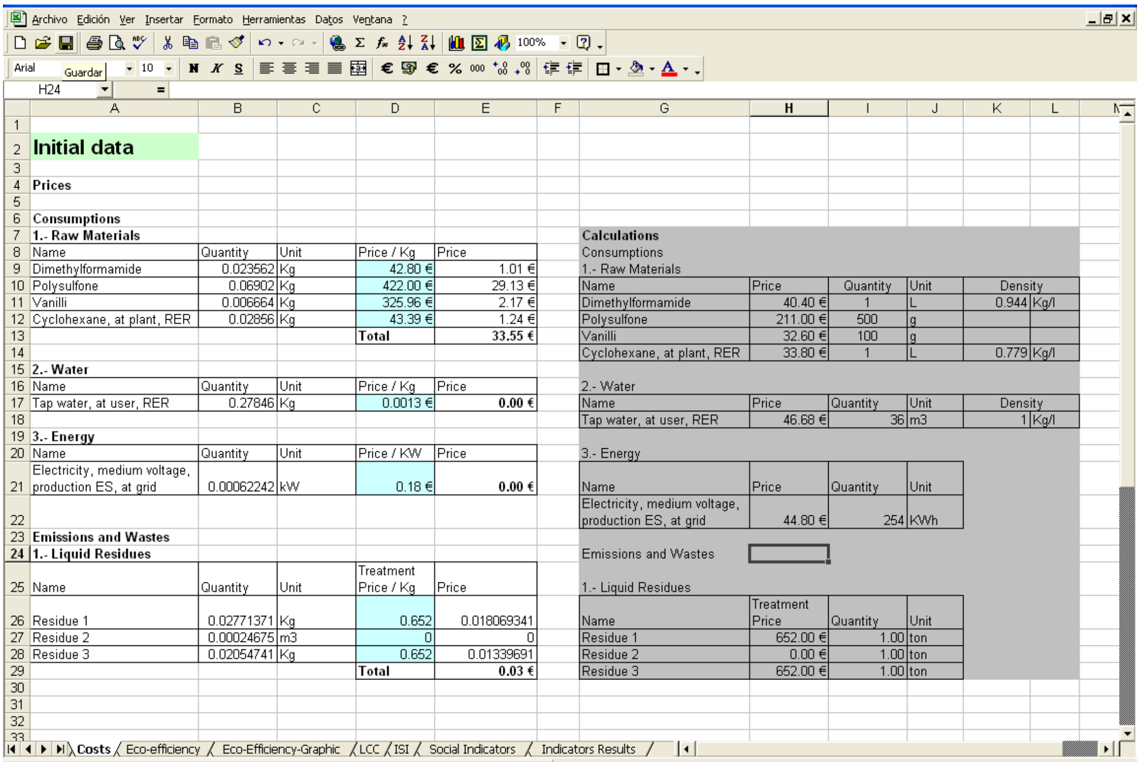


K5 = ='Calculation 1'!K5*'Characterization Factors'!$L9

Abiotic Resource Depletion ADP

Name	Category	Sub-Category	Trimethylamine, at plant, RER	Bisphenol A, powder, at plant, RER	Chemicals organic, at plant, GLO
Acetaldehyde	air	high population density	0	0	0
Acetaldehyde	air	low population density	0	0	0
Acetaldehyde	air	low population density, long-term	0	0	0
Acetaldehyde	air	lower stratosphere + upper troposphere	0	0	0
Acetaldehyde	air	unspecified	0	0	0
Acetic acid	air	high population density	0	0	0
Acetic acid	air	low population density	0	0	0
Acetic acid	air	low population density, long-term	0	0	0
Acetic acid	air	lower stratosphere + upper troposphere	0	0	0
Acetic acid	air	unspecified	0	0	0
Acetic acid, trifluoro-	air	high population density	0	0	0
Acetic acid, trifluoro-	air	low population density	0	0	0
Acetic acid, trifluoro-	air	low population density, long-term	0	0	0
Acetic acid, trifluoro-	air	lower stratosphere + upper troposphere	0	0	0
Acetic acid, trifluoro-	air	unspecified	0	0	0
Acetone	air	high population density	0	0	0
Acetone	air	low population density	0	0	0
Acetone	air	low population density, long-term	0	0	0
Acetone	air	lower stratosphere + upper troposphere	0	0	0
Acetone	air	unspecified	0	0	0
Acrolein	air	high population density	0	0	0
Acrolein	air	low population density	0	0	0
Acrolein	air	low population density, long-term	0	0	0
Acrolein	air	lower stratosphere + upper troposphere	0	0	0
Acrolein	air	unspecified	0	0	0
Actinides, radioactive, unspecified	air	high population density	0	0	0
Actinides, radioactive, unspecified	air	low population density	0	0	0

Figure 24. Environmental Impacts Calculations Data Sheets



Initial data

Prices

Consumptions

1.- Raw Materials

Name	Quantity	Unit	Price / Kg	Price
Dimethylformamide	0.023562	Kg	42.80 €	1.01 €
Polysulfone	0.06902	Kg	422.00 €	29.13 €
Vanilli	0.006664	Kg	325.96 €	2.17 €
Cyclohexane, at plant, RER	0.02856	Kg	43.39 €	1.24 €
			Total	**33.55 €**

2.- Water

Name	Quantity	Unit	Price / Kg	Price
Tap water, at user, RER	0.27846	Kg	0.0013 €	**0.00 €**

3.- Energy

Name	Quantity	Unit	Price / KW	Price
Electricity, medium voltage, production ES, at grid	0.00062242	kW	0.18 €	**0.00 €**

Emissions and Wastes

1.- Liquid Residues

Name	Quantity	Unit	Treatment Price / Kg	Price
Residue 1	0.02771371	Kg	0.652	0.018069341
Residue 2	0.00024675	m3	0	0
Residue 3	0.02054741	Kg	0.652	0.01339691
			Total	**0.03 €**

Calculations

Consumptions

1.- Raw Materials

Name	Price	Quantity	Unit	Density	
Dimethylformamide	40.40 €	1	L	0.944	Kg/l
Polysulfone	211.00 €	500	g		
Vanilli	32.60 €	100	g		
Cyclohexane, at plant, RER	33.80 €	1	L	0.779	Kg/l

2.- Water

Name	Price	Quantity	Unit	Density	
Tap water, at user, RER	46.68 €	36	m3	1	Kg/l

3.- Energy

Name	Price	Quantity	Unit
Electricity, medium voltage, production ES, at grid	44.80 €	254	KWh

Emissions and Wastes

1.- Liquid Residues

Name	Treatment Price	Quantity	Unit
Residue 1	652.00 €	1.00	ton
Residue 2	0.00 €	1.00	ton
Residue 3	652.00 €	1.00	ton

Figure 25. Economical Impacts Calculations Data Sheets

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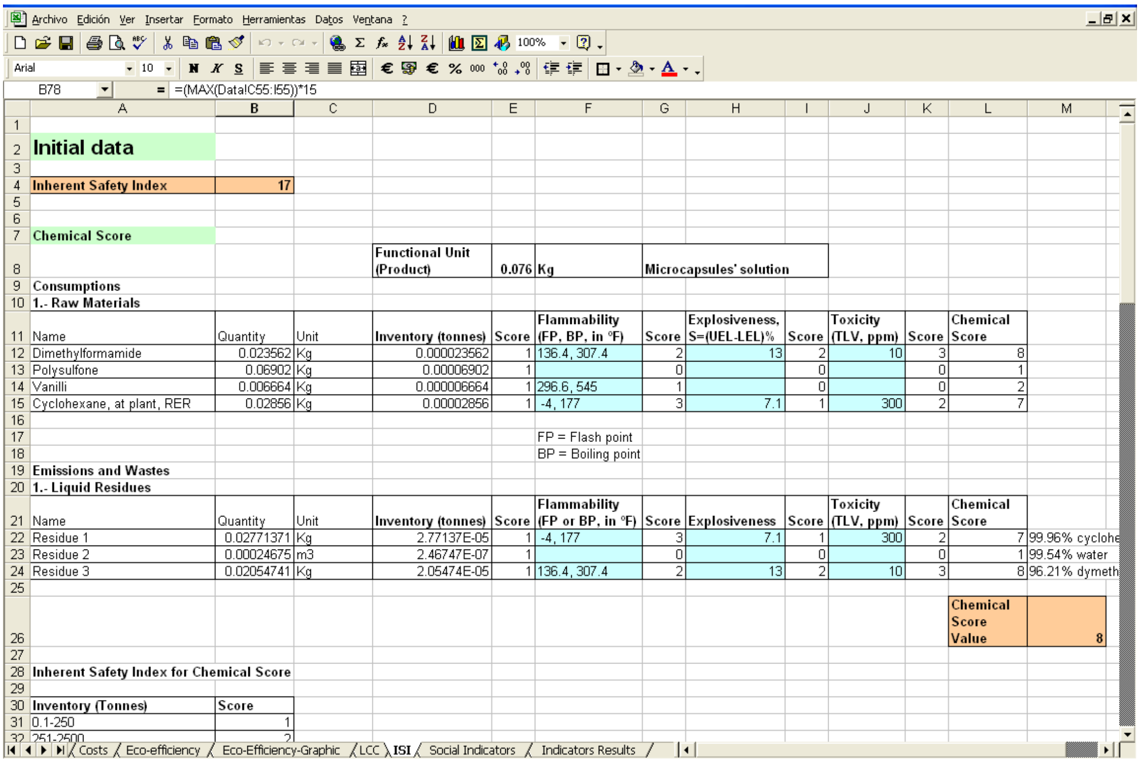


Figure 26. Inherent Safety Index Calculation Data Sheet

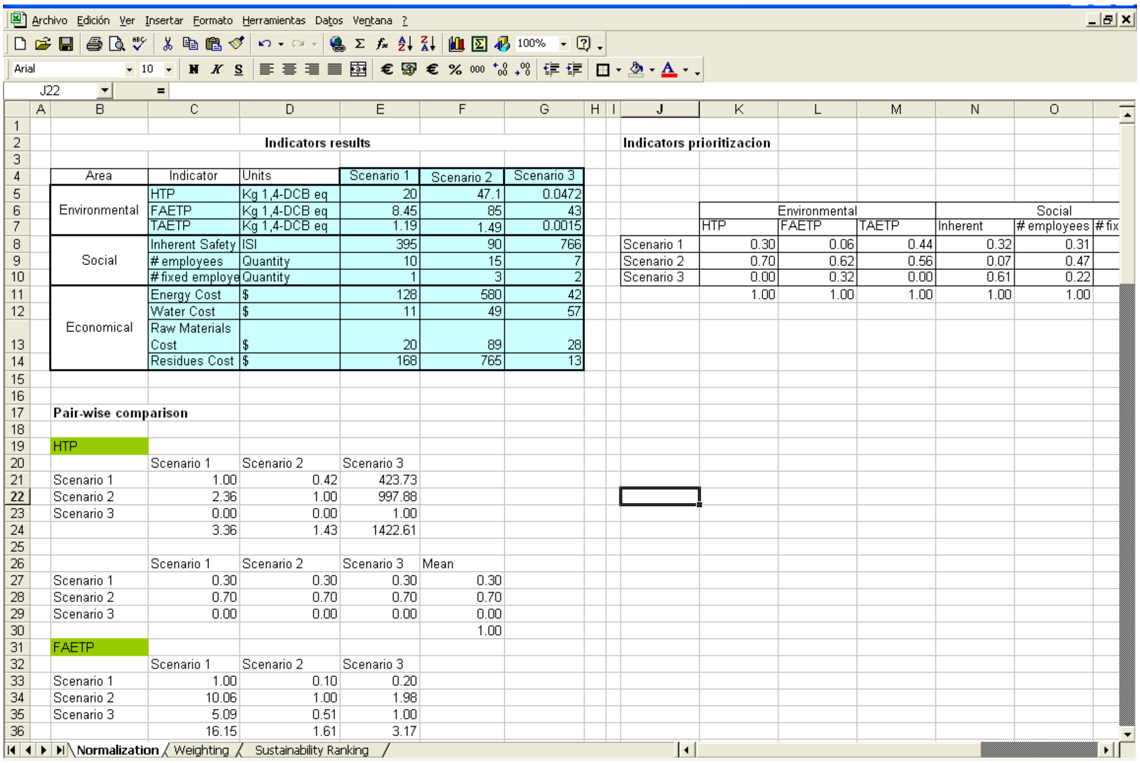
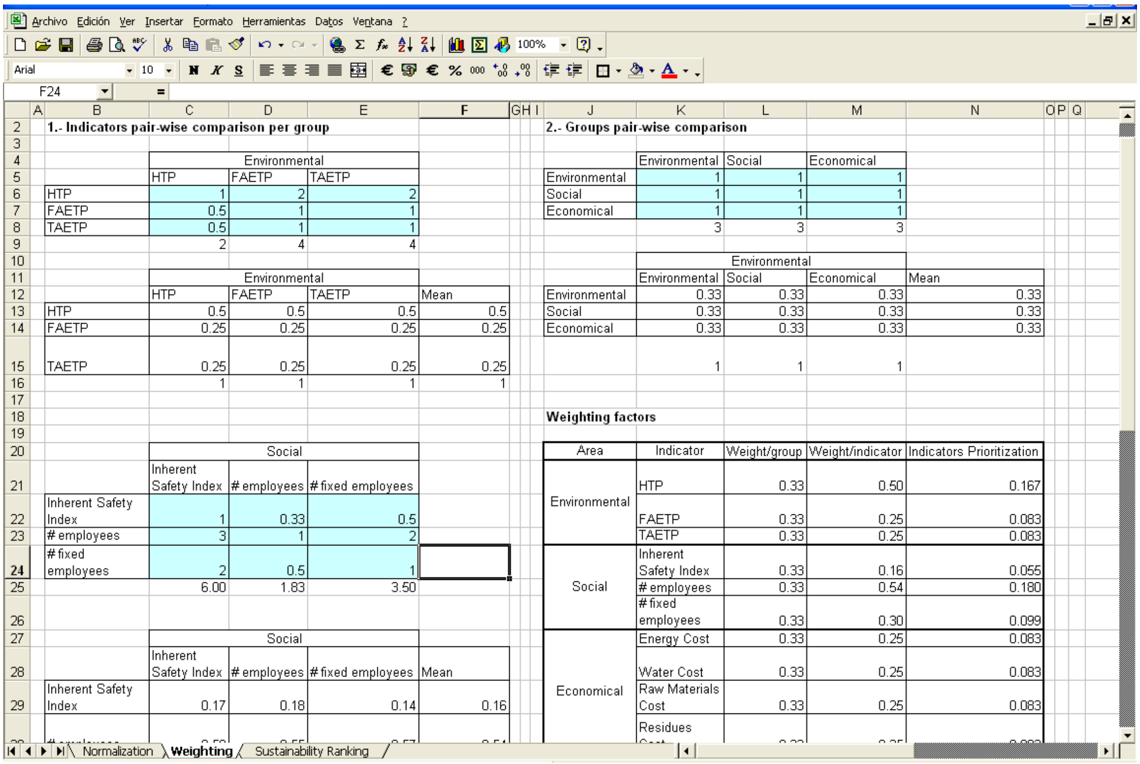


Figure 27. Indicators Prioritization Calculation Data Sheet



1.- Indicators pair-wise comparison per group

	Environmental HTP	FAETP	TAETP
HTP	1	2	2
FAETP	0.5	1	1
TAETP	0.5	1	1
	2	4	4

	Environmental HTP	FAETP	TAETP	Mean
HTP	0.5	0.5	0.5	0.5
FAETP	0.25	0.25	0.25	0.25
TAETP	0.25	0.25	0.25	0.25
	1	1	1	1

	Social Inherent Safety Index	# employees	# fixed employees
Inherent Safety Index	1	0.33	0.5
# employees	3	1	2
# fixed employees	2	0.5	1
	6.00	1.83	3.50

	Social Inherent Safety Index	# employees	# fixed employees	Mean
Inherent Safety Index	0.17	0.18	0.14	0.16

2.- Groups pair-wise comparison

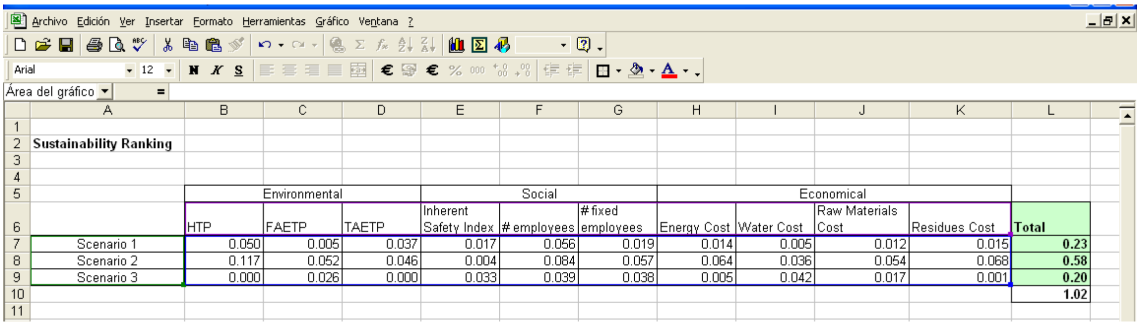
	Environmental	Social	Economical
Environmental	1	1	1
Social	1	1	1
Economical	1	1	1
	3	3	3

	Environmental	Social	Economical	Mean
Environmental	0.33	0.33	0.33	0.33
Social	0.33	0.33	0.33	0.33
Economical	0.33	0.33	0.33	0.33
	1	1	1	

Weighting factors

Area	Indicator	Weight/group	Weight/indicator	Indicators Prioritization
Environmental	HTP	0.33	0.50	0.167
	FAETP	0.33	0.25	0.083
	TAETP	0.33	0.25	0.083
Social	Inherent Safety Index	0.33	0.16	0.055
	# employees	0.33	0.54	0.180
	# fixed employees	0.33	0.30	0.099
Economical	Energy Cost	0.33	0.25	0.083
	Water Cost	0.33	0.25	0.083
	Raw Materials Cost	0.33	0.25	0.083
	Residues Cost			

Figure 28. Weighting Factors Calculation Data Sheet



Sustainability Ranking

	Environmental HTP	FAETP	TAETP	Social Inherent Safety Index	# employees	# fixed employees	Economical Energy Cost	Water Cost	Raw Materials Cost	Residues Cost	Total
Scenario 1	0.050	0.005	0.037	0.017	0.056	0.019	0.014	0.005	0.012	0.015	**0.23**
Scenario 2	0.117	0.052	0.046	0.004	0.084	0.057	0.064	0.036	0.054	0.068	**0.58**
Scenario 3	0.000	0.026	0.000	0.033	0.039	0.038	0.005	0.042	0.017	0.001	**0.20**
											1.02

Figure 29. Sustainability Ranking Calculation Data Sheet

Interpretation

In this step, a spiderplot graphic was plotted with the information obtained from the Life Cycle Impact Assessment (see Figure 20).

8.2. MICAP software

MICAP was developed by IMPULSE partner ETSEQ-URV within T3.2, with the purpose of simulating the "Production of perfume-containing microcapsules"[6] including new multi-scale design technology.

[6] Study provided by IMPULSE partner ETSEQ-URV within T3.2 (reported in D3.2c and D3.2f).

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MICAP is a deployed simulator that performs the microcapsule synthesis. It is programmed with Mathworks© Matlab© with three different simulation levels: molecular simulation, Computational Fluid Dynamics (CFD) simulation, and process simulation made with the commercial process simulator ASPEN©.

In order to compare sustainability of different production scenarios within the MICAP, a module (see Figure 30) for sustainability evaluation was created based on the Microsoft® Excel® sheets where the SLCM methodology was translated.

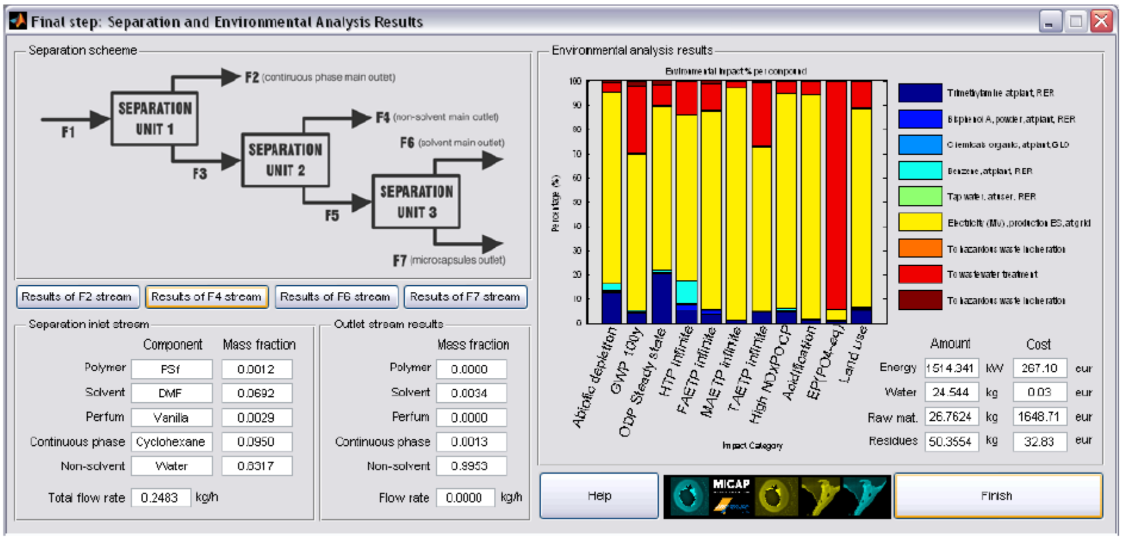

Figure 30. Example of Environmental Calculations within MICAP

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Jennifer Navarro Rosa
ISBN:978-84-692-4159-2/DL.T-1175-2009

Chapter 4. Case Study 1: Technology Comparison

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1. Introduction

To demonstrate and test the SLCM methodology, it was applied to a case study in order to determine the feasibility and data availability. The case is based on a study provided and developed by IMPULSE partner ETSEQ-URV within T3.2, "Production of perfume-containing microcapsules" (reported in D3.2c and D3.2f).

Perfume microcapsules (PMCs) are of great interest to the softener industry as they offer a mechanism for the efficient deposition of perfumes as well as providing long-lasting fragrance benefits. Perfume deposition onto fabrics is an exceptionally inefficient process as over 90 % of perfume added to a softener is lost during washing. Perfumes have to be very fabric substantive and this limits the possible fragrances.

Encapsulation of perfume into a microcapsule helps deposition because – with careful control of capsule size – the capsules become entrapped into a fabric during washing and resist being flushed away. The capsules then provide a long-lasting, consumer relevant benefit.

At the present PMCs are commercially made using interfacial polymerisation with melamine-formaldehyde (MF). This process happens in bulk and takes many hours and uses environmentally unattractive materials (esp. formaldehyde). Capsule robustness is not ideal and storage stability of commercially made MF capsules is mostly marginal.

The manufacture of a system that would allow the rapid production of smaller quantities of high integrity PMCs without the use of formaldehyde is attractive. What would be most attractive would be a system capable of making PMCs on-line with softener manufacture. The typical production run for a softener brand is now often less than one hour so any PMC making process would have to be very flexible. Micro-reactors seem to offer this possibility.

Perfumes are very complex materials. Even a simple perfume may contain 30 – 40 different components. Procter and Gamble commonly use about 200 different components in perfume making and up to 1000 components in total can be used.

These components are selected for their different characteristics. Some components are very volatile, others are not volatile. Some components are hydrophobic and some are hydrophilic. Chemically the range is very wide with alcohols, esters, and aldehydes being most common. This means that it is very hard to encapsulate some components in an aqueous system such as MF.

Therefore, a research group of ETSEQ-URV within T3.2 IMPULSE project had developed a process for production of perfume-containing microcapsules using micro-devices. The description of this production process is explained in the following section.

2. Description of Case Study 1: Technology Comparison

The encapsulation process is Phase Inversion Precipitation (described in detail in D3.2c).

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The process occurs in two phases where two micro-devices are used. In the first one, an emulsion containing polymeric and perfume droplets (with non-size dispersion) is prepared from two inlet streams. One inlet stream includes the polymeric solution containing the polymer (polysulfone or PSf), solvent (Dimethyl formamide or DMF) and perfume and the other, the continuous phase (cyclohexane). The continuous phase is immiscible with the solvent and does not act as non-solvent for the polymer. The emulsion is then used to feed the second micro-device which contains also a second inlet with the non-solvent (water), and therefore, precipitation of the polymer occurs inside it. Microcapsules are then obtained (non-size dispersion) with perfume encapsulated inside. The process is shown schematically in Figure 31.

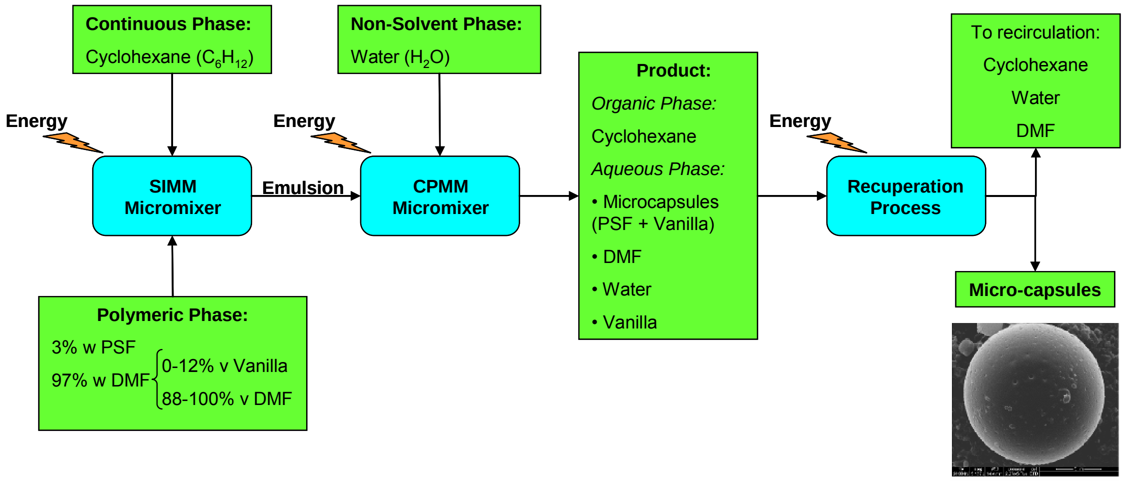

Figure 31. Micro-encapsulation process

Product's flow has to be separated in order to use the microcapsules in the production process of softeners and to reuse raw materials in the micro-encapsulation process. For this reason, a three phase's recuperation process was fit after the micro-encapsulation production process. In the first phase, a decanter is used and the recuperation of cyclohexane occurs at 97.17% (F2). In the second phase, the decanter's output flow (F3) is treated in a filter, where a 100% of solid microcapsules recuperation occurs (F7). The third phase has been evaluated by two different techniques:

- Distillation tower separation process (DTSP): the filter's output flow (F5) is treated in a distillation tower where the recuperation of water (F4) and DMF (F6) occurs. A flow diagram of this process is shown in Figure 32.

- Combined distillation-pervaporation separation process (CDPSP): the filter's output flow (F5) is treated in a distillation tower where the separation of water (F4) and DMF (F6) occurs. The DMF flow (F6) is treated in a set of three pervaporators. A flow diagram of the whole process is shown in Figure 33 while a detail of the pervaporation units is shown in Figure 34.

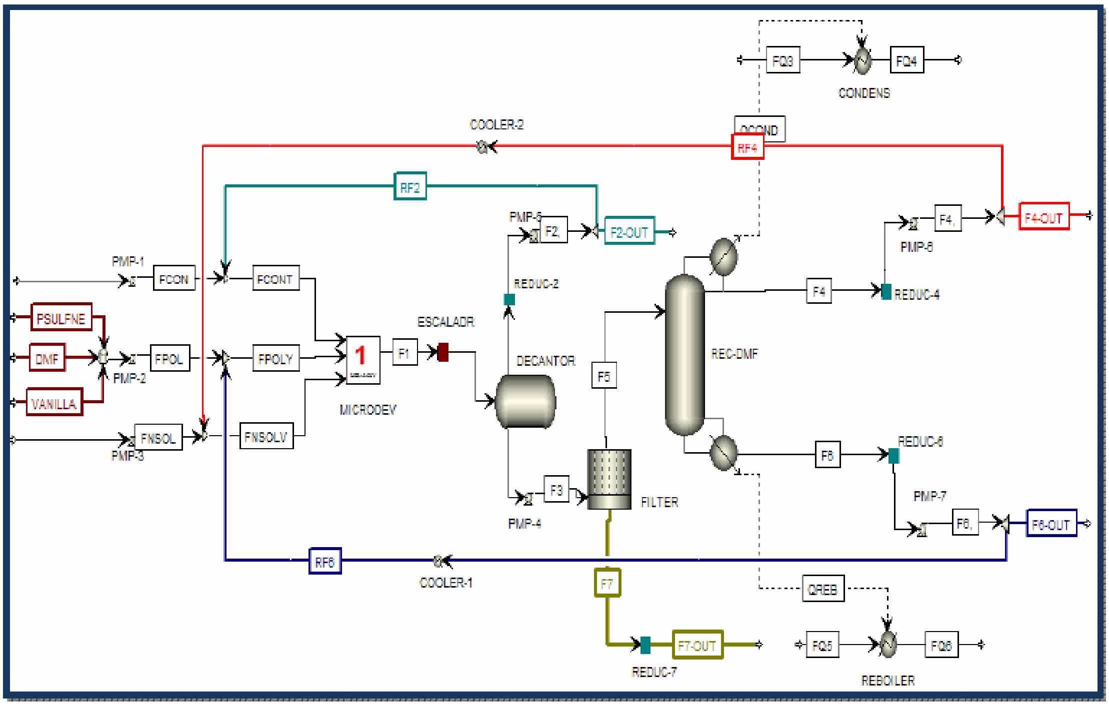

Figure 32. Micro-capsules recuperation process with distillation tower. Block 1 represents the micro-devices

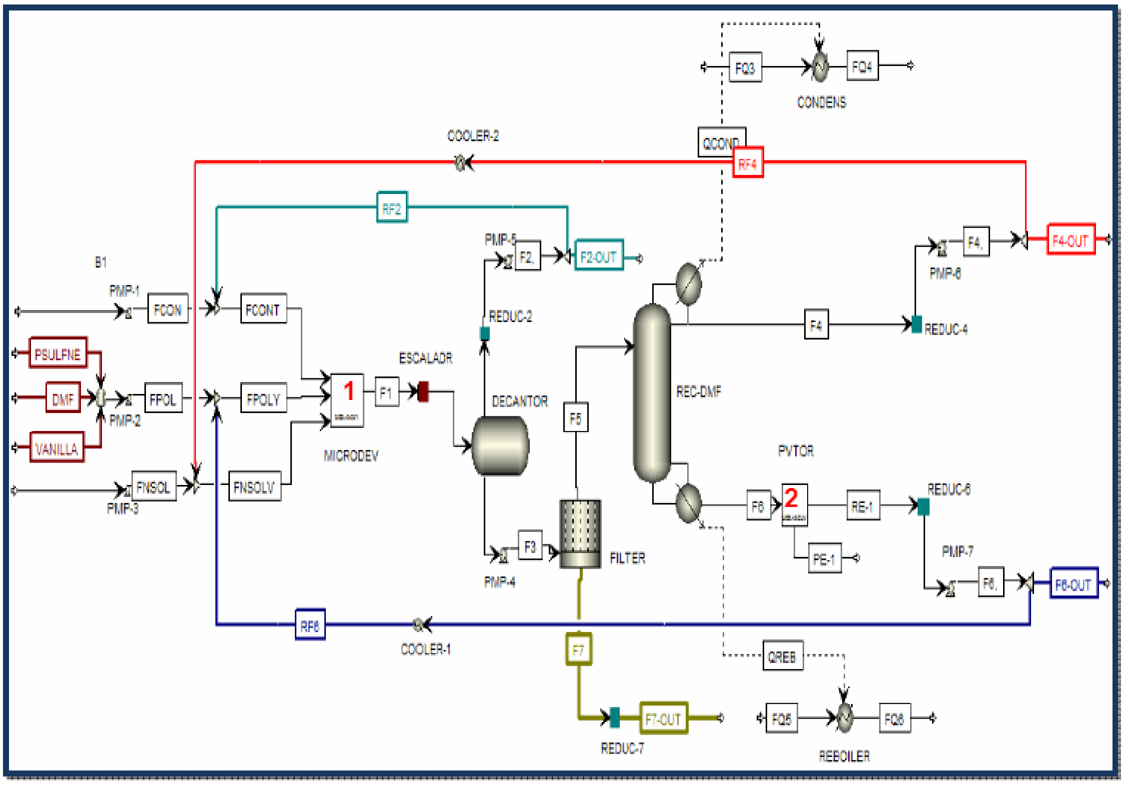

Figure 33. Micro-capsules recuperation process with combined distillation-pervaporation. Block 1 represents the micro-devices. Block 2 represents the pervaporation units

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Commercial softeners usually contain less than 5% perfume, most of which is lost during wash (about 90%), leaving less than 0,5% of perfume onto fabrics. Considering that the micro-capsules contain about 10% perfume, and that the amount of perfume that should be released onto fabrics will be of about 0,5%, the amount of micro-capsules that will be added to the softener will be lower than 5%. The perfume containing micro-capsules are then included in softeners production. After the softeners are bottled, they are distributed and sell to final user. Different feasible scenarios have been taken into account in order to calculate the corresponding sustainability profile by applying SLCM methodology, and analyze the results for all different options.

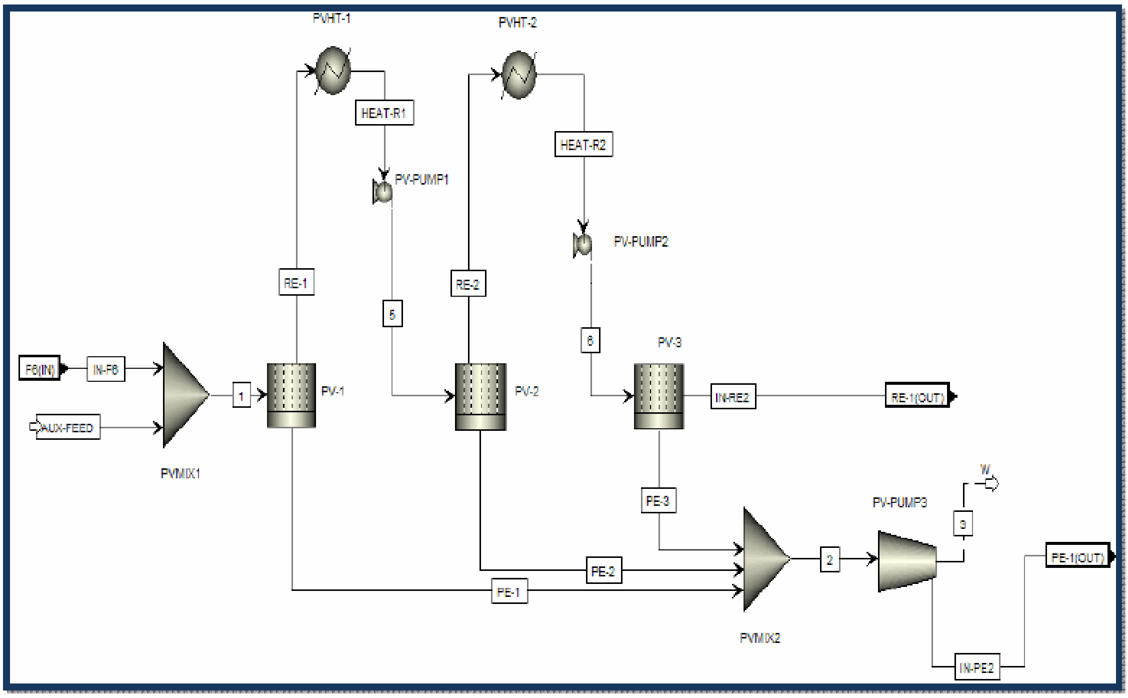

Figure 34. Pervaporation unit's detail

3. Analysis of Case Study 1

The sustainability profile of the production of perfume-containing microcapsules was obtained following the SLCM methodology described in Figure 21.

3.1. Goal & Scope Definition

The goal of the analysis of the case study is to evaluate the global sustainability profile of the perfume-containing microcapsules production process, to identify the individual parts of the technology that generate the highest impacts and to compare different scenarios for production and distribution of the product.

The *functional unit* was defined according to the micro-devices production. According to data obtained from simulations with MICAP, and in agreement with other partners from the project, the functional unit was taken as the micro-capsules production obtained from the operation of 238 micro-devices working in parallel during 1 hour.

Thus the functional unit considered within this study is the production of 0,073 kg/h micro-capsules.

The *system boundaries* were defined according to the perfume-containing microcapsules production process detailed in Figure 31.

For the operation conditions we have compared the two separation techniques used, DTSP and CDPSP.

To perform the environmental assessment, we have considered as inputs, the consumption of reactives, water and energy, and as outputs, the amount of wastes generated and their final treatment disposal. The transport of reactives to the plant and of wastes to their final destinations was also included in the study. Thus, the operation of the plant was studied in detail. However, the infrastructure of the plant, including the building and equipment, as well as the building dismantling at its end of life, were not considered within the environmental evaluation, as these stages are usually reported as negligible when compared to the operation of industrial plants (Lassaux et al., 2007; Vidal et al., 2002).

To perform the economical assessment, we have considered the initial investment costs (building infrastructure and plant equipments) and the operational costs (personnel, raw materials, transport, energy and waste disposal).

To perform the social assessment we have considered the operation of the plant, in relation with its personnel and safety considerations.

3.2. Inventory Analysis

Using data provided by process simulations with MICAP and ASPEN, and from interactions with IMPULSE partner ETSEQ-URV within T3.2, we have obtained the input and output data on energy and materials related to the functional unit that is the production of 0,073 kg/h micro-capsules, operating with 238 micro-devices in parallel. Table 13, Table 14 and Table 15 present the inventory fluxes obtained for the environmental, economical and social assessments, respectively.

The economical analysis was separated between laboratory and industrial scale. For the laboratory scale we have considered the initial investment and operation costs for a plant operating 238 micro-devices in parallel, 24 hours/day and 350 days/year. For the industrial scale we have considered the initial investment and operation costs for a plant producing the amount of microcapsules needed to cover 20% of Spanish softener demand, that is 778 blocks of 238 micro-devices each, producing a total of 56,79 kg/h. Building acquisition prices have been obtained from estate agency offers for industrial buildings located in different industrial areas of Spain. Price (800 €/m^2) was estimated as an average between different locations and building sizes. The size of the building was calculated considering the following assumptions:

- Micro-devices blocks: each block of 238 microdevices occupies a 50 cm wide / 20 cm deep area (0,1 m^2), with a 240 cm height. The same area was estimated for the accessory equipment (pumps, syringes, valves, control devices, etc.) and

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the technicians operation. Thus, a 0,3 m^2 area is estimated for each microdevices block. When several blocks are operated, the blocks are lined to form corridors of 10 m length (20 blocks).

Table 13. Inventory fluxes for environmental analysis

Name	Quantity for DTSP	Quantity for CDPSP	Unit
Raw materials			
Dimethylformamide	4,27E-02	4,27E-02	kg
Polysulfone	6,90E-02	6,90E-02	kg
Vanilli	9,16E-03	9,16E-03	kg
Cyclohexane	5,57E-02	5,57E-02	kg
Water	5,00E-01	5,00E-01	kg
Energy			
Pumping PMP-1	2,26E-07	2,26E-07	kWh
Pumping PMP-2	1,64E-07	1,64E-07	kWh
Pumping PMP-3	1,61E-06	1,61E-06	kWh
Pumping PMP-4	6,86E-04	6,86E-04	kWh
Pumping PMP-5*	-9,10E-06	-9,10E-06	kWh
Pumping PMP-6*	-1,27E-04	-1,27E-04	kWh
Pumping PMP-7*	-6,03E-06	-6,01E-06	kWh
Pervaporation PUMP1	-	4,36E-05	kWh
Pervaporation PUMP2	-	4,28E-05	kWh
Pervaporation PUMP3	-	6,58E-01	kWh
Pumping total	5,46E-04	6,58E-01	kWh
Services			
Water for cooling	1,00E+03	9,10E+02	kg/h
Steam for reboiler	5,00E+02	4,50E+02	kg/h
Wastes			
Cyclohexane	5,50E-02	5,50E-02	kg
Wastewater	4,90E-04	4,90E-04	m^3
DMF	4,30E-02	4,40E-02	kg
Transport			
Small truck (< 3,5 tn)	5,60E-02	5,60E-02	tkm

*: The negative sign of the energy values is related to the equations defined for energy balances in the Aspen simulation.

- Raw materials and final products storage: the area needed to store the raw materials was estimated by calculating the volume of reactives consumed by each block, a storage height of 240 cm and a minimum stock to operate during 30 days. The same area was estimated for the final products storage.
- Separation process: the area needed for the separation units (distillation towers and pervaporation racks) and the accessory equipment was estimated as the double of the area needed for storage.
- Offices, locking rooms and social areas: the area needed for personnel was estimated considering an office space for each 4 engineers, a changing room space for every 4 technicians and additional areas for directives offices, meeting rooms, reception desks, cafeteria, etc.
- Considering that industrial buildings available in the Spanish market usually occupy about 100 m^2 area, we have estimated that small plants will require a minimum of 100 m^2.

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For the calculation of the micro-devices costs, we have obtained prices from commercial micro-devices (www.micronit.com), and estimated a reduction in price due to the high amount of micro-devices needed. The pumps and accessory equipment for the micro-devices were also calculated per block of 238 micro-devices.

The costs of personnel were obtained from average salaries of workers in Spain, and the quantity was calculated considering that a superior engineer is required for every 20 micro-devices blocks. Also, three shifts will be performed by the technicians, and an extra technician is needed to cover weekends and holydays. Thus, a group of 4 technicians will be required every 20 micro-devices blocks.

Prices for raw materials were obtained from suppliers (Sigma Aldrich, Panreac, Sharlab, BASF).

Electricity and water prices were taken from Spanish local companies, considering Spanish prices.

The cost of wastes management was obtained from the Catalan Wastes Agency.

Costs of transport were obtained from the Ministry of Public Works from Spain and RENFE Company.

Table 14. Inventory fluxes for economical analysis

Name	Price laboratory scale	Price industrial scale	Unit
Initial investment			
Building acquisition	80.000	587.520	€
Plant equipments	3,94E+05	2,25E+08	€
Operation costs			
Personnel			
Superior engineer (quantity)	46.040 (1)	1.795.560 (39)	€/year
Technicians (quantity)	114.004 (4)	3.904.637 (137)	€/year
Raw materials			
Dimethylformamide	42,80	1,50	€/kg
Polysulfone	422,00	13,00	€/kg
Vanilli	325,96	23,62	€/kg
Cyclohexane	43,39	0,92	€/kg
Tap water	0,0013	0,0013	€/kg
Energy			
Electricity	0,18	0,18	€/kW
Wastes treatment			
Cyclohexane	0,652	0,652	€/kg
Wastewater	0,00	0,00	€/kg
DMF	0,652	0,652	€/kg
Transport			
Small truck (< 3,5 tn)	1,55	-	€/tn km
Big truck (> 16 tn)	-	0,18	€/tn km
Additional information			
Building dimensions	100	734	m^2
Micro-devices number	238	185.164	units
Microcapsules production	0,073	56,79	kg/h

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Table 15. Inventory fluxes for social analysis

Name	Quantity
Number of employees	5
Number of fixed employees	4
Number of woman employees	2
Number of foreign employees	2
Inherent safety index	17
Chemical score	8
Process score	9

In order to obtain the inherent safety index (ISI), the Chemical and Process Score were calculated following the procedure explained on Annex 5. Calculation Method for Inherent Safety Index (ISI). The data used for these calculations is shown on Table 16 for the Chemical Score and on Table 17 for the Process Score.

Table 16. Data to calculate Chemical Score Value for Perfume contained Micro-capsules case study

Name	Inventory	Score	Flammability (FP[7], BP[8], in ºF)	Score	Explosiveness, S=(UEL[9]-LEL[10])%	Score	Toxicity (TLV[11], ppm)	Score	Chemical Score
Dimethylformamide	4,27E-02 Kg	1	136.4, 307.4	2	13	2	10	3	8
Polysulfone	6,90E-02 Kg	1		0		0		0	1
Vanilli	9,16E-03 Kg	1	296.6, 545	1		0		0	2
Cyclohexane	5,57E-02 Kg	1	-4, 177	3	7,1	1	300	2	7
Residue 1 (99.96% cyclohexane)	5,542E-05 Kg	1	-4, 177	3	7,1	1	300	2	7
Residue 2 (99.54% water)	4,9E-07 m^3	1		0		0		0	1
Residue 3 (96.21% dymethylformamide)	4,3E-05 Kg	1	136.4, 307.4	2	13	2	10	3	8
								Chemical Score Value	**8**

Table 17. Data to calculate Process Score Value for Perfume contained Micro-capsules case study

	Data	Process Score
Maximum Temperature (ºC)	159,42	2
Maximum Pressure (psi)	18	1
% yield	41,29	6
Process Score Value		**9**

Hypothesis and assumptions

Electricity mix: for electricity consumptions we have used environmental information on the Spanish electrical mix (composition described in Table 18).

[7] FP = Flash Point
[8] BP = Boiling Point
[9] UEL= Upper Explosive Limit
[10] LEL= Lower Explosive Limit
[11] TLV= Threshold Limit Value

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Table 18. Spanish electricity mix (data taken from ecoinvent V2.01 database)

Electricity type	Contribution (%)
Coal	24,3
Lignite	3,7
Oil	8,4
Natural gas	19,6
Industrial gas	0,4
Hydropower	12,7
Nuclear	22,8
Photovoltaic	0,1
Wind	5,8
Wood	1,5
Biogas	0,6

Use of eco-vectors and proxies: environmental information for all the fluxes considered in the inventory was obtained from ecoinvent V2.01 (2007) database. In those cases where the environmental information about a product or process was not found within the ecoinvent database, we have selected a proxy instead, considering that it should be a product or process with similar characteristics. The eco-vectors and proxies used are described in Table 19.

Table 19. Inventory fluxes for environmental analysis

Name	Database eco-vectors	Comments
Dimethylformamide	N,N-dimethylformamide, at plant	The eco-vector describes the production of DMF from dimethylamine in Europe including materials, energy uses, infrastructure and emissions. Raw materials are modelled with a stoechiometric calculation. Energy consumptions are modelled with literature data. The emissions are estimated. Infrastructure and transports are calculated with standard values.
Polysulfone	Bisphenol A, powder, at plant	Polysulfone data were not available within the ecoinvent database. Bisphenol A, a monomer used in the synthesis of polysulfone, was used instead. The eco-vector includes the raw materials and chemicals used for production, transport of materials to manufacturing plant, estimated emissions to air and water from production (incomplete), estimation of energy demand and infrastructure of the plant (approximation). Solid wastes were omitted.
Vanilli	Chemicals organic, at plant	Vanilli data were not available within the ecoinvent database. A mixture of organic components was used instead. A general module for organic chemicals is established, based on the modules of several organic substances from the ecoinvent database. An unweighted average of the first 20 organic substances, being part of the top100 chemicals and included into this database, is established.
Cyclohexane	Cyclohexane, at plant	The eco-vector includes the production of cyclohexane including materials, energy uses, infrastructure and emissions. The process is modelled for the production of cyclohexane from benzene in Europe
Water	Tap water, at user	The eco-vectors include the infrastructure and energy use for water treatment and transportation to the end user
Electricity	Electricity, medium voltage, production	The eco-vector includes the electricity production in Spain, the transmission network and direct SF6-emissions to air.

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	ES, at grid	Electricity losses during medium-voltage transmission and transformation from high-voltage are accounted for.
Water cooler	Water, completely softened, at plant	The eco-vector includes the use of chemicals and some emissions for the treatment of water used in power plants.
Steam reboiler	Steam, for chemical processes, at plant	The eco-vector includes the input of water and energy for the production of steam. No further infrastructure is included, as the heating infrastructure is part of the respective heating modules used.
Residue 1: Ciclohexane	Disposal, solvents mixture, 16.5% water, to hazardous waste incineration	The eco-vector includes the waste-specific air and water emissions from incineration, auxiliary material consumption for flue gas cleaning. Short-term emissions to river water and long-term emissions to ground water from residual material landfill (from solidified fly ashes and scrubber sludge).
Residue 2: Wastewater	Treatment, maize starch production effluent, to wastewater treatment, class 2	The eco-vector includes the infrastructure materials for municipal wastewater treatment plant, transports, dismantling. Wastewater is purified in a moderately large municipal wastewater treatment plant (capacity class 2), with an average capacity size of 71100 per-capita-equivalents PCE.
Residue 3: DMF	Disposal, solvents mixture, 16.5% water, to hazardous waste incineration	The eco-vector includes the waste-specific air and water emissions from incineration, auxiliary material consumption for flue gas cleaning. Short-term emissions to river water and long-term emissions to ground water from residual material landfill (from solidified fly ashes and scrubber sludge).
Transport		
Small truck (< 3,5 tn)	Transport, van <3.5t	The eco-vector includes the operation of the vehicle; production, maintenance and disposal; construction and maintenance and disposal of road. Inventory refers to the entire transport life cycle.
Big truck (> 16 tn)	Transport, lorry >16t, fleet average	The eco-vector includes the operation of the vehicle; production, maintenance and disposal; construction and maintenance and disposal of road. Inventory refers to the entire transport life cycle.
Train	Transport, freight, rail	The eco-vector includes the operation, production, maintenance and disposal of vehicles and construction, maintenance and disposal of railway tracks. Inventory refers to the entire transport life cycle.

3.3. Indicators selection

Environmental area

The impact categories selected for the environmental evaluation were those described within the CML2001 baseline methodology:

- Depletion of abiotic resources (ADP) in kg antimony-Eq
- Climate change (GWP) in kg CO_2-Eq
- Stratospheric ozone depletion (ODP) in kg CFC-11-Eq
- Human toxicity (HTP) in kg 1,4-DCB-Eq
- Freshwater aquatic ecotoxicity (FAETP) in kg 1,4-DCB-Eq
- Marine aquatic ecotoxicity (MAETP) in kg 1,4-DCB-Eq
- Terrestrial ecotoxicity (TAETP) in kg 1,4-DCB-Eq
- Photochemical oxidation (POCP) in kg ethylene-Eq

- Acidification potential (AP) in kg SO_2-Eq
- Eutrophication potential (EP) in kg PO_4-Eq
- Land use in m^2year

Economic area

The impact categories selected for the economic evaluation were those included within the eco-efficiency indicators, together with some LCC indicators:

- Raw materials cost
- Energy costs
- Water cost
- Residues treatment cost
- Initial investment
- Operation cost

Social area

The impact categories selected for the social evaluation were a combination of indicators related to the worker situation (such as ratio between fixed and temporal employees), the health and safety (such as the inherent safety index), and the gender and diversity equities.

3.4. Life Cycle Impact Assessment

Environmental area

Results for the DTSP and CDPSP are summarised in Table 20 and Table 21 respectively. It can be observed that both processes have similar total values for their environmental impacts. In both cases the use of services (specially the use of steam at the reboilers), is the major contributor to the environmental impact. Differences between both processes are mainly related to the pumping energy, because of the three extra pumps used in the pervaporation process in CDPSP.

Table 20. Environmental LCA for DTSP

Impact category	Units	Raw materials	Pumping energy	Services	Wastes	Transport	Total
ADP	kg antimony-Eq	7,37E-03	2,09E-06	9,42E-01	1,60E-04	7,57E-04	8,56E-01
GWP	kg CO2-Eq	5,65E-01	2,86E-04	1,17E+02	1,35E-01	1,10E-01	1,06E+02
ODP	kg CFC-11-Eq	2,42E-08	1,55E-11	1,44E-05	3,24E-09	1,51E-08	1,30E-05
HTP	kg 1,4-DCB-Eq	1,17E+00	7,49E-05	3,12E+01	7,27E-03	3,58E-02	2,93E+01
FAETP	kg 1,4-DCB-Eq	1,72E-01	1,81E-05	2,23E+00	4,78E-03	6,93E-03	2,19E+00
MAETP	kg 1,4-DCB-Eq	1,21E+02	3,04E-01	2,06E+04	9,89E+00	2,38E+01	1,87E+04
TAETP	kg 1,4-DCB-Eq	1,22E-03	1,28E-06	6,44E-01	1,65E-04	3,93E-04	5,81E-01
POCP	kg ethylene-Eq	3,20E-04	9,95E-08	1,50E-02	3,60E-06	4,00E-05	1,38E-02
AP	kg SO2-Eq	1,96E-03	2,70E-06	2,79E-01	1,04E-04	4,14E-04	2,54E-01
EP	kg PO4-Eq	3,90E-03	1,38E-07	1,62E-02	2,52E-04	6,78E-05	1,88E-02
Land use	m2y	7,84E-03	7,43E-06	1,45E-01	4,56E-04	3,67E-03	1,43E-01

Table 21. Environmental LCA for CDPSP

Impact category	Units	Raw materials	Pumping energy	Services	Wastes	Transport	Total
ADP	kg antimony-Eq	7,37E-03	2,51E-03	8,47E-01	1,61E-04	7,57E-04	8,58E-01
GWP	kg CO2-Eq	5,65E-01	3,45E-01	1,05E+02	1,36E-01	1,10E-01	1,06E+02
ODP	kg CFC-11-Eq	2,42E-08	1,87E-08	1,29E-05	3,26E-09	1,51E-08	1,30E-05
HTP	kg 1,4-DCB-Eq	1,17E+00	9,03E-02	2,80E+01	7,32E-03	3,58E-02	2,94E+01
FAETP	kg 1,4-DCB-Eq	1,72E-01	2,19E-02	2,00E+00	4,82E-03	6,93E-03	2,21E+00
MAETP	kg 1,4-DCB-Eq	1,21E+02	3,67E+02	1,86E+04	9,97E+00	2,38E+01	1,91E+04
TAETP	kg 1,4-DCB-Eq	1,22E-03	1,55E-03	5,79E-01	1,66E-04	3,93E-04	5,83E-01
POCP	kg ethylene-Eq	3,20E-04	1,20E-04	1,35E-02	3,63E-06	4,00E-05	1,40E-02
AP	kg SO2-Eq	1,96E-03	3,26E-03	2,52E-01	1,05E-04	4,14E-04	2,57E-01
EP	kg PO4-Eq	3,90E-03	1,66E-04	1,46E-02	2,52E-04	6,78E-05	1,90E-02
Land use	m2y	7,84E-03	8,95E-03	1,31E-01	4,60E-04	3,67E-03	1,52E-01

The contribution of every flux considered in the inventory to the total impact is reflected in Figure 35 and Figure 36, for the DTSP and CDPSP scenarios respectively. From both figures it can be concluded that the steam used in the reboiler is the major cause of the environmental impact, with a contribution higher than 95% in most of the categories studied, except for the freshwater aquatic ecotoxicity, the eutrophication potential and the land use. These results reflect the need of improvement for the separation process, in order to reduce the amount of steam needed.

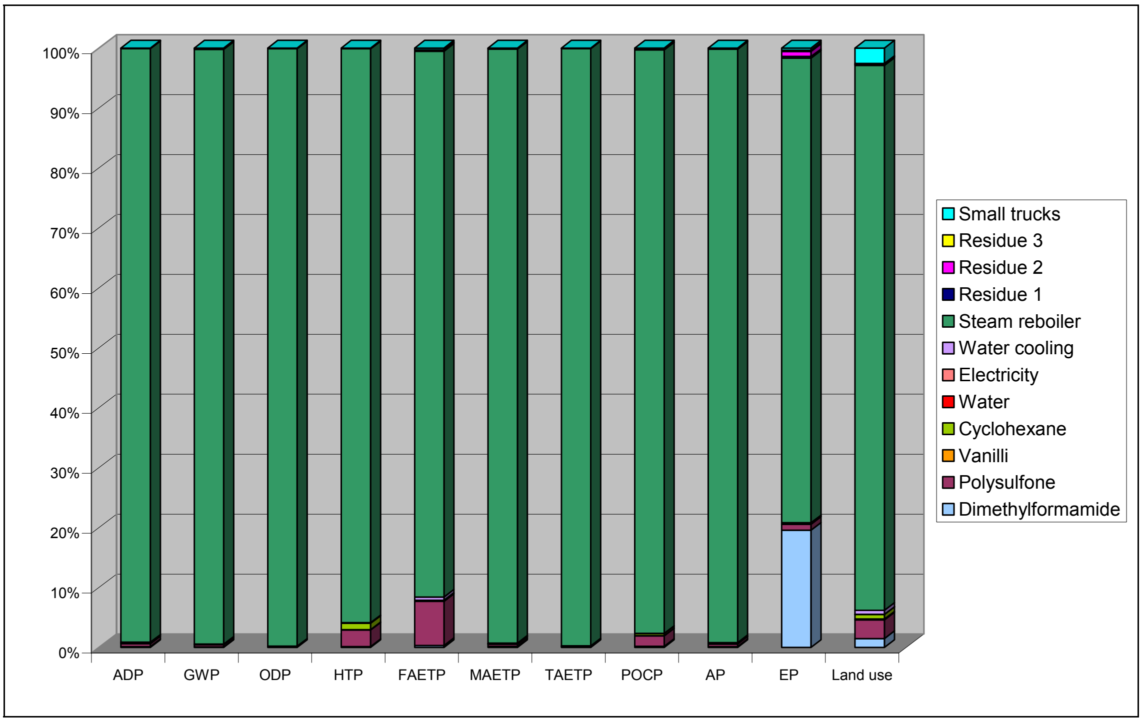

Figure 35. Environmental LCA for DTSP. Percentage contributions.

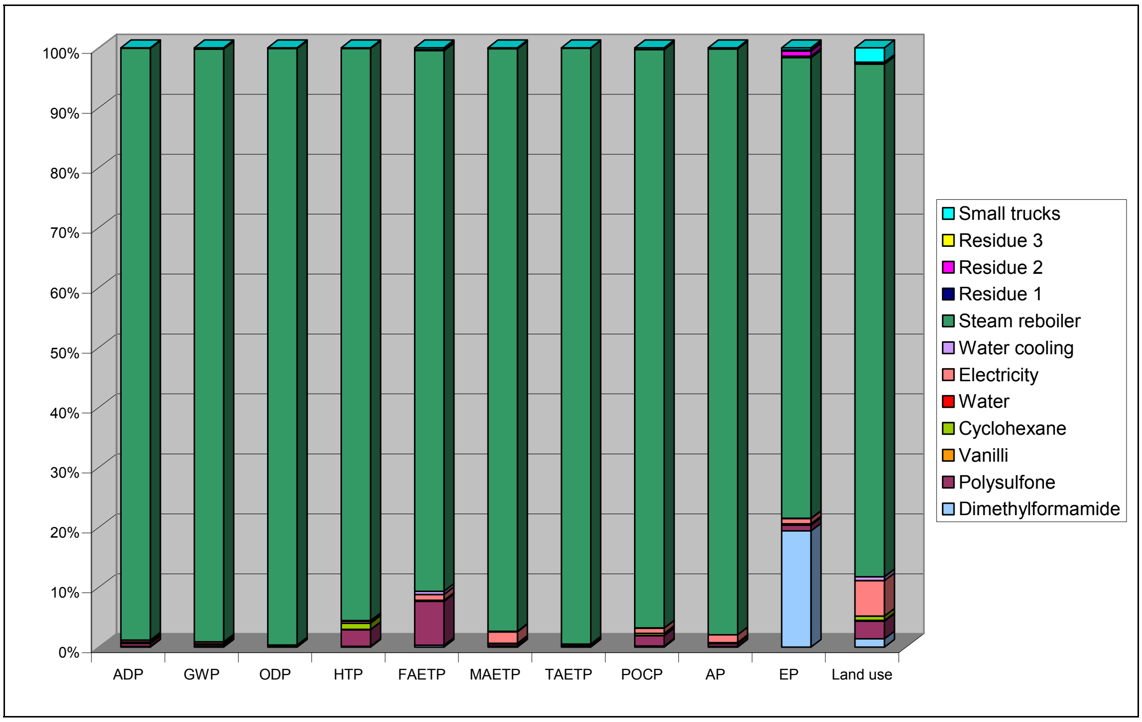

Figure 36. Environmental LCA for CDPSP. Percentage contributions.

In order to have a clearer comparison of the different fluxes involved in the process, Figure 37 and Figure 38 present the LCA results for the DTSP and CDPSP scenarios respectively, excluding the impact of the services (steam and cooling water).

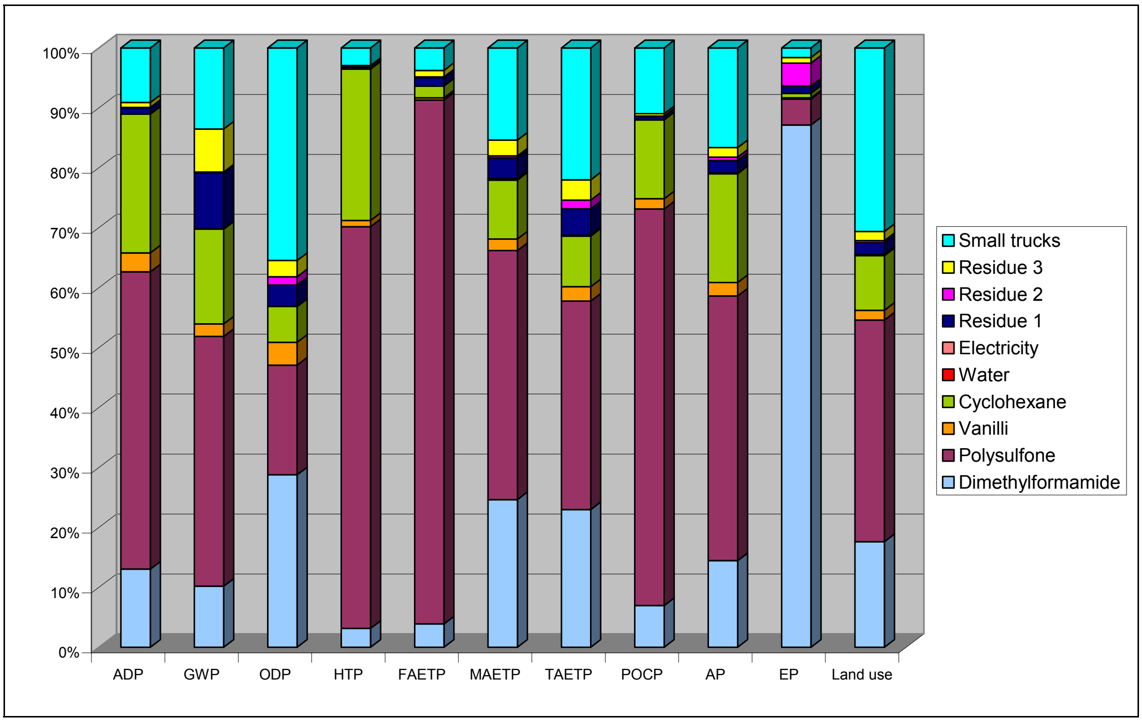

Figure 37. Environmental LCA for DTSP. Percentage contributions excluding services.

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In the case of the distillation tower separation process (DTSP), we observe that the use of polysulfone (followed by dimethylformamide, cyclohexane and the transport), is the major contribution to most of the environmental impact categories, specially the case of the human toxicity, freshwater aquatic ecotoxicity and photochemical oxidation. The production of dimethylformamide is the major contribution to eutrophication. The impact of the production of vanilli, the use of water, the wastes disposal and the pumping energy, are negligible in most of the categories.

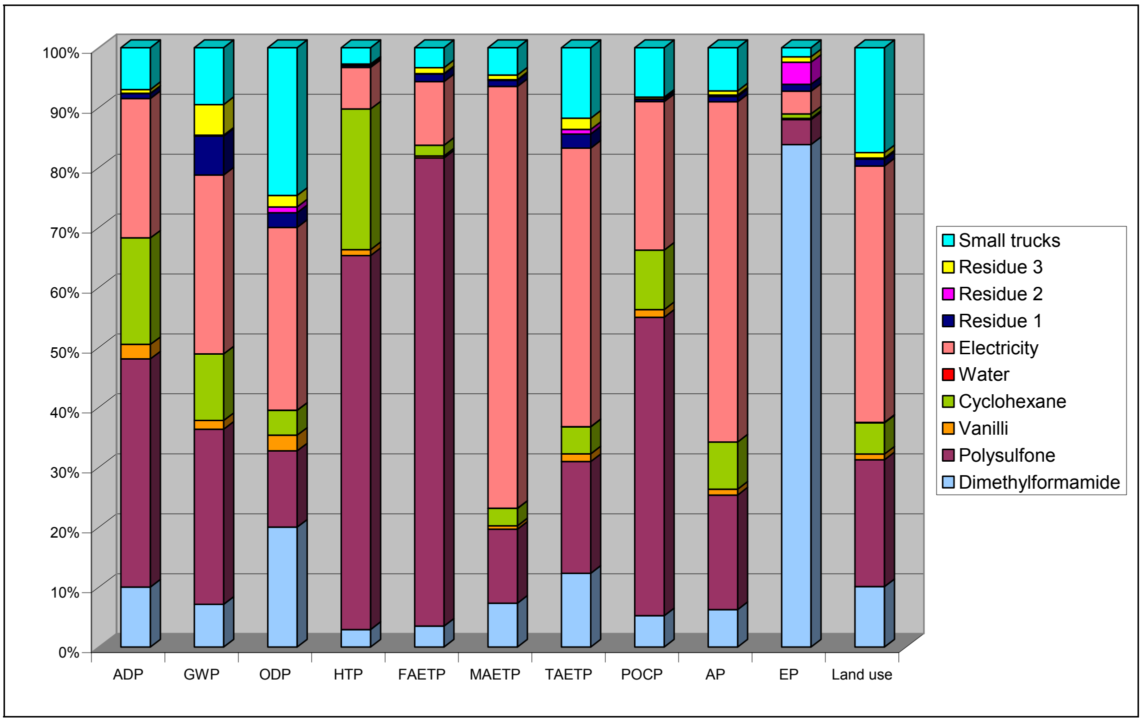

Figure 38. Environmental LCA for CDPSP. Percentage contributions excluding services.

In the case of the combined distillation-pervaporation separation process (CDPSP), we observe similar results than those of DTSP. However, the electricity for pumping is higher in this scenario, due to the extra pumps necessary for the pervaporation process, thus causing a major contribution of this flux in the total environmental impacts.

Economic area

A comparison of the economical costs of producing microcapsules at laboratory or industrial scale was made, considering the use of blocks of 238 micro-devices each, from the production of the functional unit to the Spanish demand covering. Results are presented in Table 22, where the operation costs are compared. In Figure 39 the evolution of the different operation costs can be observed in terms of production scale.

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Table 22. LCC comparison for laboratory and industrial scale operation

	Laboratory scale	Industrial scale	Unit
Personnel	239	11	€/functional unit
Raw materials	36,36	5,32	€/functional unit
Energy	1,74	1,74	€/functional unit
Water	1,95	1,95	€/functional unit
Residues disposal	0,06	0,06	€/functional unit
Investment amortization	61	45	€/functional unit

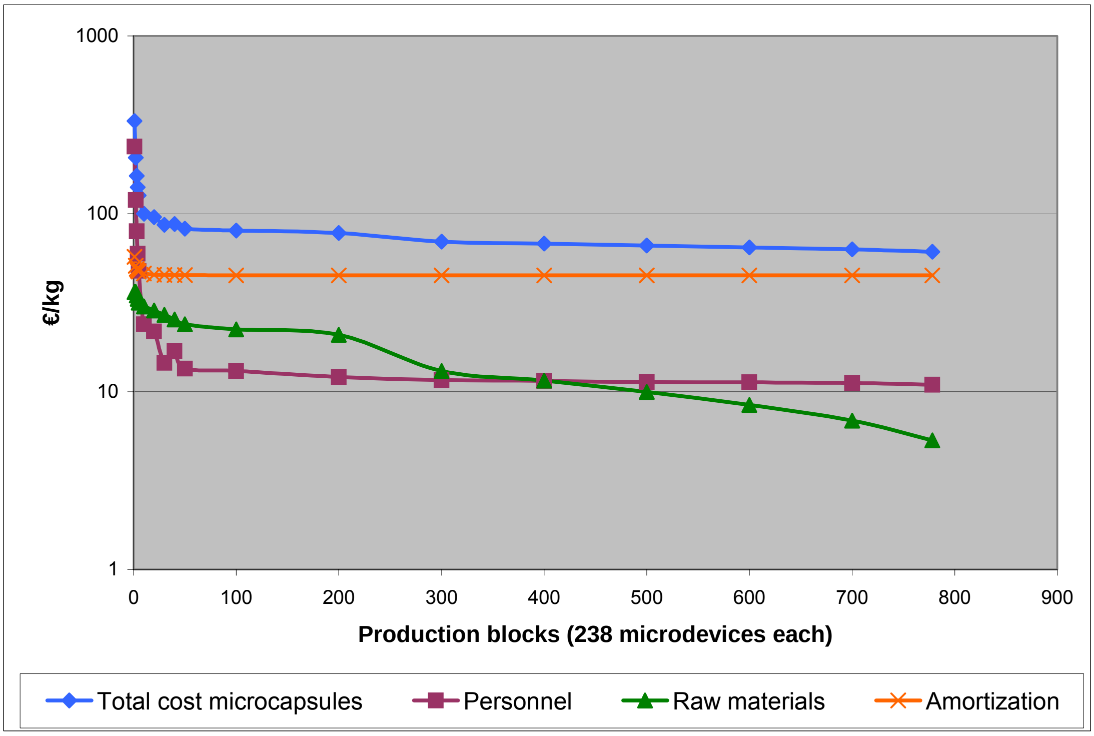

Figure 39. Operation costs for microcapsules production at different scales

From the analysis of the inventory data, and the cost for the initial investment amortization, it can be concluded that the cost of the micro-devices is the critical point within the initial investment, due to the number of micro-devices needed to be operating in parallel to cover the demand and the high cost of each individual micro-device and accessories.

Social area

Social indicators were compared (Table 23) for the operation of the plant at laboratory or industrial scale, considering the use of blocks of 238 micro-devices each, from the production of the functional unit to the Spanish demands covering.

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Table 23. Social impact assessment

Name	Laboratory scale	Industrial scale
Number of employees	5	176
Number of superior engineers	1	39
Number of technicians	4	137
Number of fixed employees	4	142
Fixed employees proportion	0,8	0,81
Number of woman employees	2	88
Woman employees proportion	0,4	0,5
Number of foreign employees	2	88
Foreign employees proportion	0,4	0,5
Inherent safety index	17	17

3.5. Indicators aggregation

The main advantage of the methodology is that it allows comparison between different processes. Thus, we have compared the two different scenarios for separation of products (DTSP and (CDPSP), with a process were no separation was considered. Then we have three different cases:

- Case 1: perfume-containing microcapsules production process excluding the use of services (cooling water and steam) for the separation of the products.
- Case 2: perfume-containing microcapsules production process including the products separation by means of a distillation tower (DTSP).
- Case 3 perfume-containing microcapsules production process including the products separation by means of a combined distillation-pervaporation process (CDPSP).

A sustainability index was obtained by aggregating the results from the environmental, economic and social impact assessments. This process was performed in five different stages, as explained in the methodology chapter.

For the first stage, indicators prioritization and normalization, the indicators to be compared were selected:

- Environmental assessment: Human toxicity, freshwater aquatic ecotoxicity and terrestrial ecotoxicity
- Social assessment: Inherent safety index, number of employees and number of fixed employers.
- Economic assessment: costs of energy, water, raw materials and wastes treatments costs

Table 24 to Table 31 presents the indicators aggregation steps to obtain the sustainability index for the three case studies.

Table 24. Indicators results

Area	Indicator	Units	Case 1	Case 2	Case 3
Environmental	HTP	Kg 1,4-DCB eq	1,21	32,38	29,35
	FAETP	Kg 1,4-DCB eq	0,18	2,41	2,21
	TAETP	Kg 1,4-DCB eq	0,0018	0,65	0,58
Social	Inherent Safety Index	ISI	17	17	17
	# employees	Quantity	4	5	5
	# fixed employees	Quantity	3	4	4
Economical	Energy Cost	$	0,0001	1,74	1,77
	Water Cost	$	0,0006	1,95	1,76
	Raw Materials Cost	$	36,36	36,36	36,36
	Residues Cost	$	0,06	0,06	0,06

Table 25. Indicators prioritization

	Environmental			**Social**			**Economical**			
	HTP	FAETP	TAETP	Inherent Safety Index	# employees	# fixed employees	Energy Cost	Water Cost	Raw Materials Cost	Residues Cost
Case 1	0,02	0,04	0,00	0,33	0,29	0,27	0,00	0,00	0,33	0,39
Case 2	0,51	0,50	0,52	0,33	0,36	0,37	0,50	0,52	0,33	0,39
Case 3	0,47	0,46	0,47	0,33	0,36	0,37	0,50	0,48	0,33	0,22
	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00

A comparison between indicators not together but per groups was made. In the environmental area (Table 26), the same weigh was given to FAETP and to TAETP due to the proximity and contact between the Medias. Same weigh were given to these indicators than to the HTP, according to the weighting procedure of Eco-indicator 99.

Table 26. Environmental Weighting Calculation

	Environmental		
	HTP	FAETP	TAETP
HTP	1	2	2
FAETP	0.5	1	1
TAETP	0.5	1	1
	2	4	4

	Environmental			
	HTP	FAETP	TAETP	Mean
HTP	0.5	0.5	0.5	0.5
FAETP	0.25	0.25	0.25	0.25
TAETP	0.25	0.25	0.25	0.25
	1	1	1	1

In the social aspects (Table 27), the same weigh was given to all indicators, since they were considered equally important.

Table 27. Social Weighting Calculation

	Social		
	Inherent Safety Index	# employees	# fixed employees
Inherent Safety Index	1	1	1
# employees	1	1	1
# fixed employees	1	1	1
	3	3	3

	Social			
	Inherent Safety Index	# employees	# fixed employees	Mean
Inherent Safety Index	0.33	0.33	0.33	0.33
# employees	0.33	0.33	0.33	0.33
# fixed employees	0.33	0.33	0.33	0.33
	1.00	1.00	1.00	1.00

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For the economic area (Table 28), the same weigh was given to all indicators, since they are all measure in the same unit (€).

Table 28. Economical Weighting Calculation

	Economical			
	Energy Cost	Water Cost	Raw Materials Cost	Residues Cost
Energy Cost	1	1	1	1
Water Cost	1	1	1	1
Raw Materials Cost	1	1	1	1
Residues Cost	1	1	1	1
	4	4	4	4

	Economical				
	Energy Cost	Water Cost	Raw Materials Cost	Residues Cost	Mean
Energy Cost	0.25	0.25	0.25	0.25	0.25
Water Cost	0.25	0.25	0.25	0.25	0.25
Raw Materials Cost	0.25	0.25	0.25	0.25	0.25
Residues Cost	0.25	0.25	0.25	0.25	0.25
	1	1	1	1	1

Then, a comparison between the groups of indicators was made (Table 29). The same weigh was assigned to each group. So, a 0.33 was given to each one. It is important to note that the weighs can vary according to the case study.

Table 29. Indicators Group Weighting Calculation

	Environmental	Social	Economical
Environmental	1	1	1
Social	1	1	1
Economical	1	1	1
	3	3	3

	Environmental	Social	Economical	Mean
Environmental	0.33	0.33	0.33	0.33
Social	0.33	0.33	0.33	0.33
Economical	0.33	0.33	0.33	0.33
	1	1	1	1

After the calculations, the indicators prioritization was obtained. The weigh per groups was multiplied per the weigh per indicator to obtain the indicators prioritization (Table 30).

Table 30. Indicators weighting factors

Area	**Indicator**	**Weight/group**	**Weight/indicator**	**Indicators Prioritization**
Environmental	HTP	0,33	0,50	0,167
	FAETP	0,33	0,25	0,083
	TAETP	0,33	0,25	0,083
Social	Inherent Safety Index	0,33	0,33	0,111
	# employees	0,33	0,33	0,111
	# fixed employees	0,33	0,33	0,111
Economical	Energy Cost	0,33	0,25	0,083
	Water Cost	0,33	0,25	0,083
	Raw Materials Cost	0,33	0,25	0,083
	Residues Cost	0,33	0,25	0,083

Sustainability ranking of the indicators was obtained by multiplying the indicators prioritization per the weighting factors of each case. Table 31 shows the results obtained.

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Table 31. Sustainability ranking

	Environmental			Social			Economic				
	HTP	FAETP	TAETP	Inherent Safety Index	# employees	# fixed employees	Energy Cost	Water Cost	Raw Materials Cost	Residues Cost	Total
Case 1	0,003	0,003	0,000	0,037	0,032	0,030	0,000	0,000	0,028	0,032	**0,17**
Case 2	0,086	0,042	0,044	0,037	0,040	0,041	0,041	0,044	0,028	0,032	**0,43**
Case 3	0,078	0,038	0,039	0,037	0,040	0,041	0,042	0,040	0,028	0,019	**0,40**

From the sustainability ranking, shown in the total column, it can be concluded that the exclusion of a separation process can reduce the impact of the process and thus its sustainability index. However, no products separation means no raw materials recycling and thus higher reactives consumption and wastes generation.

The comparison of cases 2 and 3, including separation processes shows that the combined distillation-pervaporation separation process is more sustainable than the distillation separation alone. The use of pervaporation units reduces the amount of cooling water and steam at the distillation stage, while increases the energy consumption of pumping.

The differences of cases 2 and 3 with case 1 show us that the separation process is being actually the most important process in terms of sustainability. This does not mean that the separation process should be ignored but that the technology used should be optimised by reducing its energy consumptions without reducing the separation yields. This can be achieved by changes in the separation technology or by reducing the impacts associated with the actual technologies. A possible solution could be the implementation of renewable energies to obtain the steam needed for the reboilers. This process is actually performed by means of fossil fuels (according to ecoinvent database), which could be changed to alternative fuels that have lower emissions. Optimization of the process can also reduce the amount of steam needed, thus reducing its impacts.

Figure 40 presents a sustainability ranking comparison for the three analysed cases.

Figure 40 also shows us that case 1 is closer located to the centre of the diagram, thus meaning a better sustainability behaviour. On the other hand, cases 2 and 3 present similar results, slightly better for case 2.

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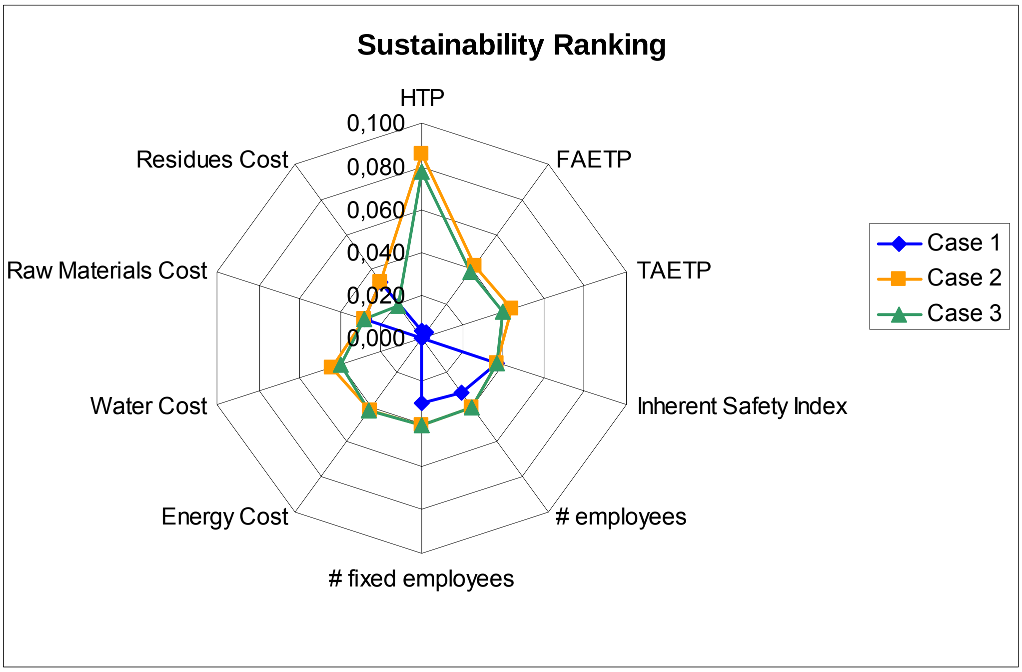

Figure 40. Triple bottom line framework

4. Conclusions for case study 1

It was demonstrated that the SLCM methodology is a suitable tool for the sustainability evaluation of the case study, allowing the comparison of different technology scenarios, production scales, and the identification of the critical points of the process (those having the highest impacts).

From the environmental evaluation it can be concluded that the critical point within the perfume-containing microcapsules production process is the use of steam at the distillation column reboiler. This result is caused by two effects: the considerably high amount of steam needed for the separation process and the use of fossil fuels to produce that steam. Having that, future efforts should be focused in the optimisation of the separation technology in order to reduce the impacts.

When comparing the rest of flows related to the process, it can be observed that the production of the raw materials (especially polysulfone) is the main responsible of the environmental impacts. The transport of raw materials and wastes has a secondary importance while the impacts of the residues final treatment and the water consumption are negligible.

When comparing the use of distillation tower, or a combination of distillation-pervaporation, it is observed that the use of pervaporation units reduces the amount of steam needed for the separation (and thus its environmental impact), while increasing the pumping energy consumption.

From the economic evaluation it can be concluded that the cost of the micro-devices is the critical point within the initial investment, due to the number of micro-devices needed to be operating in parallel to cover the demand and the high cost of each individual micro-device and accessories. The production of microcapsules at different

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production scales shows that the size of the production plant is an important parameter to consider when evaluating the production and distribution network. While the initial investment is proportional to the amount of micro-devices operating in parallel, the operating costs (especially raw materials and personnel) are reduced with the increment in the production capacity of the plant.

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Chapter 5. Case Study 2: Production Distribution Network

1. Introduction

In case study 2, the process studied in case study 1 at industrial level was taken as a basis to analyse the product distribution network of the microcapsules, including different transport media.

2. Description of Case Study 2: Product Distribution Network

In order to apply SLCM to the case study, it would be good to compare traditional technology with an intensified process including micro-scale equipment. Nevertheless, information about traditional process is not available, since the continuous production of perfume-containing microcapsules is an innovative process developed within IMPULSE Project.

In this innovative process where micro equipments are involved, it is obvious that the space used for industrial purpose will play an important role, and decentralization of industries can be considered as a good option. It can be easily translated in a comparison, from the sustainability point of view, between big enterprises with centralized production vs. dispersed production in small enterprises located in different places to supply the same region to analyze.

The product distribution network can be directly designed or optimized using Supply Chain Management (SCM) methodology. By the moment, only the directly designed product distribution network have been done and is presented bellow. The comparison of the different scenarios and the optimization of the places to locate the enterprises and distribution centres using Supply Chain Management (SCM) methodology will be finished in the near future, by means of environmental and economic data.

The following assumptions were taken into account to define the scenarios:

- Total production of perfume-containing microcapsules of a specific enterprise is used in the production of a specific washing machine softener.
- The micro encapsulation process is located close or in the same place where the specific softener is produced.
- Due to the location of the research centre and data availability, the Spanish market was selected for the analysis of the case study. Therefore, the softener and microcapsules factories will be placed in Spain.
- In order to compare different distribution sites placed around Spain, including big enterprises with centralized production vs. dispersed production in small enterprises (from the sustainability point of view), five strategic distribution centres had been selected (Figure 41).
- Since transport is going to play an important role in the proposed scenarios, distribution of softener to final sellers will be analyzed. Scenarios where big trucks and trains are used for big load transportation, from industries to distribution centres, will be analyzed. Also, scenarios where big trucks and trains are used for transportation of product, from distribution centres to final sellers, will be analyzed.

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- A total amount of 50,000 ton/year will be assumed as the quantity of equivalent softener to be perfumed with microcapsules used by the Spanish population. (To estimate this amount it was considered a 20% of market share from the total Spanish consumption of softener).
- The DTSP (case 2) and CDPSP (case 3) were taken into account to make the analysis with the different product distribution networks proposed.

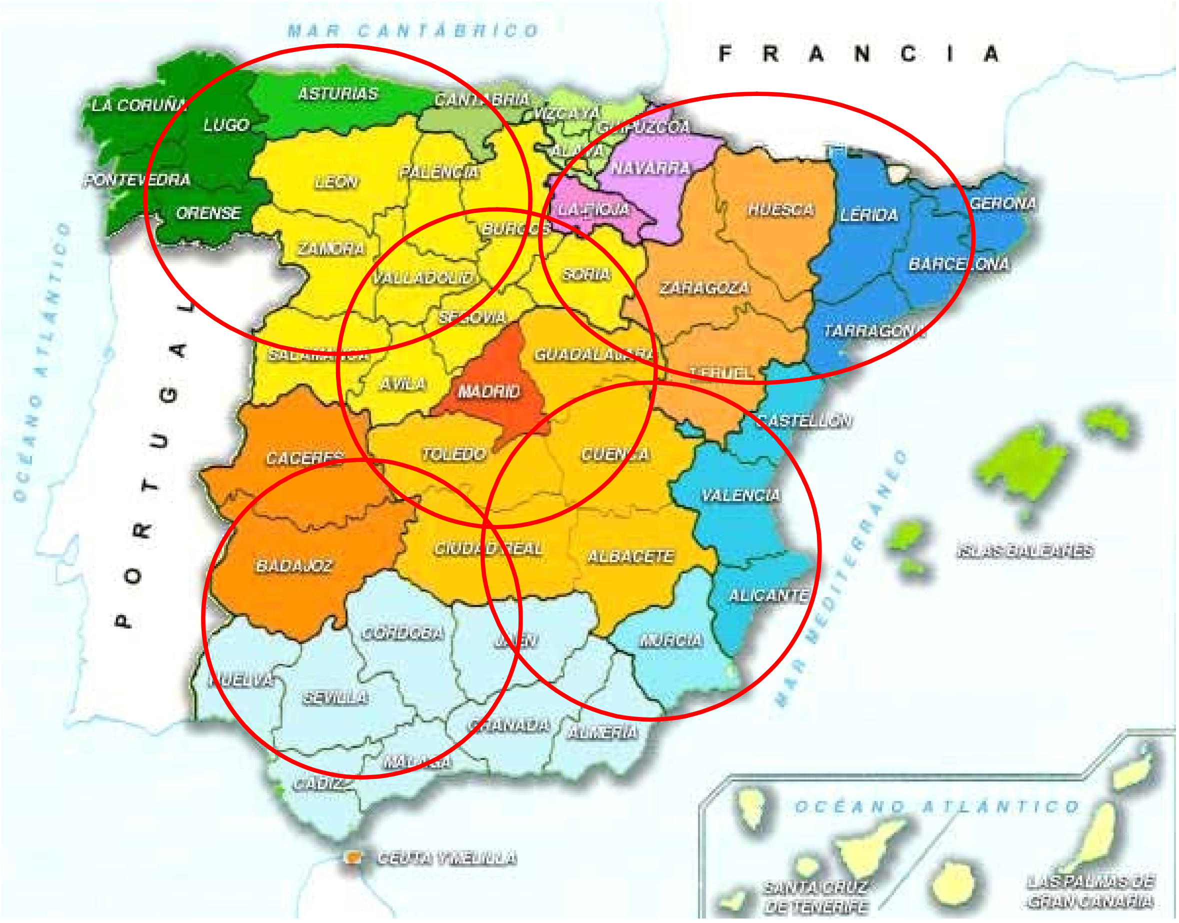

Figure 41. Strategic distribution sites in Spain

2.1. Scenario 1: one big enterprise with centralize production and big loads distributed by train to four strategic places

For scenario 1, the following assumptions have been taken into account. The big enterprise with centralize production is placed in Madrid as this is a central area of Spain. Distribution all over the country is assumed by one central (Madrid) and four regional distributions centres. Regional distributions centres receive big loads by ***train*** from headquarter (Madrid). The selected regional centres in Spain are: León, Zaragoza, Sevilla and Albacete. Distances from Madrid to regional centres are shown in Table 32. Final product is then distributed to final seller in small trucks from the five distributions centres (Madrid, León, Zaragoza, Sevilla and Albacete). Distances from distribution centres to the final sellers are shown in Table 33.

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Table 32. Distances from central area to regional distribution centres of Spain

From	To	Distance in Km	Population %
Madrid	Madrid	0	61,17
	Sevilla	535	19,48
	León	339	5,51
	Albacete	255	4,11
	Zaragoza	318	9,72

Table 33. Distances from distribution centres to final sellers in Spain

From	To	Distance in Km	Population %
Madrid	Toledo	90	1,52
	Cuenca	166	0,56
	Guadalajara	60	0,49
	Segovia	92	0,42
	Ávila	114	0,46
	Valladolid	211	1,40
	Salamanca	206	0,97
	Madrid	0	15,24
Sevilla	Huelva	92	1,30
	Cáceres	265	1,13
	Cádiz	125	3,14
	Málaga	220	3,62
	Cordoba	145	2,14
	Granada	261	2,31
	Sevilla	0	4,85
León	La Coruña	320	3,08
	Lugo	230	1,01
	Pontevedra	416	2,54
	Orense	308	0,95
	Asturias	170	2,99
	Cantabria	270	1,50
	Zamora	135	0,56
	Palencia	173	0,49
	Burgos	178	0,98
	León	0	1,37
Albacete	Jaén	282	1,81
	Ciudad Real	219	1,35
	Murcia	151	3,37
	Alicante	171	4,11
	Almería	354	1,51
	Valencia	194	6,23
	Castellón	274	1,36
	Albacete	0	1,03
Zaragoza	Tarragona	238	1,71
	Barcelona	312	13,50
	Gerona	391	1,59
	Lérida	151	1,02
	Huesca	72	0,58
	Navarra	150	1,56
	La Rioja	230	0,78
	Alava	260	0,80
	Soria	160	0,25
	Zaragoza	0	2,42
	Tarragona	238	1,71

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2.2. Scenario 2: one big enterprise with centralize production and big loads distributed by big trucks to four strategic places

For scenario 2, the following assumptions have been taken into account. The big enterprise with centralize production is placed in Madrid as this is a central area of Spain. Distribution all over the country is assumed by one central (Madrid) and four regional distribution centres. Regional distributions centres receive big loads by ***big trucks*** from headquarter (Madrid). The selected regional centres in Spain are: León, Zaragoza, Sevilla and Albacete. Distances from Madrid to regional centres are shown in Table 32. Final product is then distributed to final seller in small trucks from the five distributions centres (Madrid, León, Zaragoza, Sevilla and Albacete). Distances from distribution centres to the final sellers are shown in Table 33.

2.3. Scenario 3: disperse production in small enterprises in five different strategic places

For scenario 3, the following assumptions have been taken into account. Five small disperse production enterprises where placed in the following strategic places: Madrid, León, Zaragoza, Sevilla and Albacete. From this production places, the product will be transported by ***train*** to final sellers in big cities. Distances from distribution centres to the final sellers are shown in Table 33.

2.4. Scenario 4: disperse production in small enterprises

For scenario 4, the following assumptions have been taken into account. Five small disperse production enterprises where placed in the following strategic places: Madrid, León, Zaragoza, Sevilla and Albacete. From this production places, the product will be transported by ***big trucks*** to final sellers in big cities.

In Scenarios 1 & 2, distances from distribution centres to final seller were taken from Table 33.

3. Analysis of Case Study 2

The sustainability profile of the production of perfume-containing microcapsules at industrial scale was obtained following the SLCM methodology described in Figure 21.

3.1. Goal & Scope Definition

The goal of the analysis of the case study is to evaluate how the transport types, the location of the plants and the production type (big enterprises with centralized production vs. dispersed production in small enterprises) affect the sustainability profile of the perfume-containing microcapsules production process.

The *functional unit* was defined based on the microcapsules contained in 20 % of the annual demand of softener in Spain. Thus the functional unit considered within this

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study is the production of 500 ton/year of micro-capsules, equivalent to 1% of content of capsules in the softener.

The *system boundaries* were defined in the same way as in case study 1, with the main difference that the transport of the final product and different distribution centres was included.

For the operation conditions we have compared the two separation techniques used, DTSP and CDPSP.

To perform the environmental assessment, we have considered the results obtained from case study 1 but converted to industrial scale, and with the addition of the environmental loads produced by the transport.

To perform the economical assessment, we have considered the initial investment costs (building infrastructure and plant equipments) and the operational costs (personnel, raw materials, transport, energy and waste disposal).

To perform the social assessment we have considered the operation of the plant, in relation with its personnel and safety considerations.

3.2. Inventory Analysis

Using data provided by process simulations with MICAP and ASPEN, and from interactions with IMPULSE partner ETSEQ-URV within T3.2, we have obtained the input and output data on energy and materials related to the functional unit that is the production of 500 ton/year micro-capsules, operating with 778 blocks of 238 micro-devices each in parallel. Table 34 to Table 41 present the inventory fluxes obtained for the environmental, economical and social assessments.

Table 34. Inventory fluxes for environmental analysis of the production process

Name	Quantity for DTSP	Quantity for CDPSP	Unit
Raw materials			
Dimethylformamide	3,35E+01	3,35E+01	kg
Polysulfone	5,37E+01	5,37E+01	kg
Vanilli	7,16E+00	7,16E+00	kg
Cyclohexane	4,36E+01	4,36E+01	kg
Water	3,89E+02	3,89E+02	kg
Energy			
Pumping total	4,25E-01	5,12E+02	kWh
Services			
Water for cooling	7,78E+05	7,08E+05	kg/h
Steam for reboiler	3,89E+05	3,50E+05	kg/h
Wastes			
Cyclohexane	4,28E+01	4,28E+01	kg
Wastewater	3,81E-01	3,81E-01	m3
DMF	3,35E+01	3,42E+01	kg
Transport of raw materials and wastes			
Small truck (< 3,5 tn)	4,36E+01	4,36E+01	tkm

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Table 35. Inventory fluxes for environmental analysis of the distribution network

Transport type	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Unit
Small truck (< 3,5 tn)	87067	87067	0	0	tkm
Big truck (> 16 tn)	0	82167	0	87067	tkm
Train	82167	0	87067	0	tkm

Table 36. Inventory of micro-devices required per microcapsules production

	Distribution Centre	Microcapsules production (ton/year)	Micro-devices blocks (units)
Scenarios 1 & 2	Madrid	5,00E+02	7,78E+02
Scenarios 3 & 4	Madrid	3,06E+02	4,75E+02
	Sevilla	9,74E+01	1,52E+02
	León	2,76E+01	4,30E+01
	Albacete	2,06E+01	3,20E+01
	Zaragoza	4,86E+01	7,60E+01

Table 37, Table 38 and Table 39 are based on the information shown on Table 36.

Table 37. Inventory for required employees

	Distribution Centre	# of Engineers	# of Technicians	Total # of Employees	Fixed # of employees	Woman # of employees
Scenarios 1 & 2	Madrid	39	137	176	142	88
Scenarios 3 & 4	Madrid	24	84	108	87	54
	Sevilla	8	28	36	29	18
	León	3	11	14	12	7
	Albacete	2	7	9	8	4
	Zaragoza	4	14	18	15	9

Table 38. Inventory for initial investment

	Distribution Centre	Initial Investment (€)	Total Initial Investment (€)
Scenarios 1 & 2	Madrid	225.000.000	225.000.000
Scenarios 3 & 4	Madrid	9.360.000	226.000.000
	Sevilla	12.500.000	
	León	22.200.000	
	Albacete	44.100.000	
	Zaragoza	138.000.000	

Table 39. Inventory for cost of raw materials

	Distribution Centre	Cost of Raw Material (€/kg)	Total Cost of Raw Material (€/kg)
Scenarios 1 & 2	Madrid	5,32	5,32
Scenarios 3 & 4	Madrid	5,32	6,09
	Sevilla	5,32	
	León	6,87	
	Albacete	7,65	
	Zaragoza	5,32	

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Table 40. Inventory fluxes for economical analysis

Name	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Unit
Total initial investment	2.25E+08	2.25E+08	2.26E+08	2.26E+08	€
Operation					
Number of employees	1,76E+02	1,76E+02	1,85E+02	1,85E+02	persons
Cost of raw materials	5,32E+00	5,32E+00	6,09E+00	6,09E+00	€/kg
Energy					
Electricity	1,80E-01	1,80E-01	1,80E-01	1,80E-01	€/kW
Wastes treatment					
Cyclohexane	6,52E-01	6,52E-01	6,52E-01	6,52E-01	€/kg
Wastewater	0,00E+00	0,00E+00	0,00E+00	0,00E+00	€/kg
DMF	6,52E-01	6,52E-01	6,52E-01	6,52E-01	€/kg
Transport					
Small truck (< 3,5 tn)	1,55E+00	1,55E+00	1,55E+00	1,55E+00	€/tn km
Big truck (> 16 tn)	-	1,80E-01	-	1,80E-01	€/tn km
Train	2,30E-02	-	2,30E-02	-	€/tn km
Additional information					
Building dimensions	7,34E+02	7,34E+02	9,42E+02	9,42E+02	m^2
Micro-devices blocks	7,78E+02	7,78E+02	7,78E+02	7,78E+02	units
Microcapsules production	5,00E+02	5,00E+02	5,00E+02	5,00E+02	Ton/year

The data were obtained from the same sources as in case study 1.

Table 41. Inventory fluxes for social analysis

Name	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Number of employees	176	176	185	185
Number of fixed employees	142	142	151	151
Number of woman employees	88	88	92	92
Inherent safety index	17	17	17	17
Chemical score	8	8	8	8
Process score	9	9	9	9

Hypothesis and assumptions

Electricity mix: for electricity consumptions we have used environmental information on the Spanish electrical mix (composition described in Table 18).

Use of eco-vectors and proxies: environmental information for all the fluxes considered in the inventory was obtained from ecoinvent V2.01 (2007) database. In those cases where the environmental information about a product or process was not found within the ecoinvent database, we have selected a proxy instead, considering that it should be a product or process with similar characteristics. The eco-vectors and proxies used are described in Table 19.

3.3. Indicators selection

Environmental area

The impact categories selected for the environmental evaluation were those described within the CML2001 baseline methodology:

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- Depletion of abiotic resources (ADP) in kg antimony-Eq
- Climate change (GWP) in kg CO_2-Eq
- Stratospheric ozone depletion (ODP) in kg CFC-11-Eq
- Human toxicity (HTP) in kg 1,4-DCB-Eq
- Freshwater aquatic ecotoxicity (FAETP) in kg 1,4-DCB-Eq
- Marine aquatic ecotoxicity (MAETP) in kg 1,4-DCB-Eq
- Terrestrial ecotoxicity (TAETP) in kg 1,4-DCB-Eq
- Photochemical oxidation (POCP) in kg ethylene-Eq
- Acidification potential (AP) in kg SO_2-Eq
- Eutrophication potential (EP) in kg PO_4-Eq
- Land use in m^2year

Economic area

The impact categories selected for the economic evaluation were those included within the eco-efficiency indicators, together with some LCC indicators:

- Raw materials cost
- Energy costs
- Water cost
- Residues treatment cost
- Initial investment
- Operation cost

Social area

The impact categories selected for the social evaluation were a combination of indicators related to the worker situation (such as ratio between fixed and temporal employees), the health and safety (such as the inherent safety index), and the gender and diversity equities.

3.4. Life Cycle Impact Assessment

Environmental area

Results for the four scenarios and for the DTSP and CDPSP are summarised in Table 42. It can be observed that DTSP and CDPSP processes have similar total values for their environmental impacts. As a conclusion we observe that the options of using train for transportation, and the decentralization of production centres are more environmentally friendly.

Economic area

The results of the economical analysis are presented in Table 43.

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Social area

The results of the social indicators are shown in Table 41.

Table 42. Environmental LCA for DTSP and CDPSP

		DTSP				CDPSP			
Impact category	Units	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 1	Scenario 2	Scenario 3	Scenario 4
ADP	kg antimony-Eq	1,97E+03	2,02E+03	7,98E+02	8,54E+02	1,90E+03	1,95E+03	7,24E+02	7,80E+02
GWP	kg CO2-Eq	2,69E+05	2,76E+05	9,93E+04	1,07E+05	2,60E+05	2,67E+05	9,01E+04	9,76E+04
ODP	kg CFC-11-Eq	3,54E-02	3,68E-02	1,20E-02	1,35E-02	3,42E-02	3,57E-02	1,08E-02	1,23E-02
HTP	kg 1,4-DCB-Eq	8,32E+04	8,41E+04	2,77E+04	2,87E+04	8,07E+04	8,17E+04	2,52E+04	2,62E+04
FAETP	kg 1,4-DCB-Eq	1,31E+04	1,32E+04	2,35E+03	2,47E+03	1,29E+04	1,30E+04	2,19E+03	2,30E+03
MAETP	kg 1,4-DCB-Eq	5,57E+07	5,55E+07	1,88E+07	1,85E+07	5,44E+07	5,41E+07	1,74E+07	1,72E+07
TAETP	kg 1,4-DCB-Eq	1,15E+03	1,16E+03	5,42E+02	5,54E+02	1,10E+03	1,11E+03	4,91E+02	5,02E+02
POCP	kg ethylene-Eq	7,54E+01	7,65E+01	1,33E+01	1,44E+01	7,43E+01	7,53E+01	1,22E+01	1,33E+01
AP	kg SO2-Eq	8,90E+02	9,29E+02	2,48E+02	2,89E+02	8,70E+02	9,09E+02	2,28E+02	2,69E+02
EP	kg PO4-Eq	1,24E+02	1,34E+02	1,91E+01	2,94E+01	1,23E+02	1,33E+02	1,79E+01	2,82E+01
Land use	m2y	5,99E+03	5,99E+03	2,96E+02	3,04E+02	5,98E+03	5,99E+03	2,91E+02	3,00E+02

The main difference between the analyzed scenarios is that for scenarios 1 & 2 there is a transportation of big loads from the big enterprise with centralized production to the strategic distribution centers; while for scenarios 3 & 4 this transportation is not required. As LCA methodology analyzes the complete life cycle of the case study, all indicators results are lower for scenarios 3 & 4 than for scenarios 1 & 2 due to transport.

Table 43. Economical analysis results for DTSP and CDPSP

		DTSP				CDPSP			
		Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Investment	€ total	2,25E+08	2,25E+08	2,26E+08	2,26E+08	2,25E+08	2,25E+08	2,26E+08	2,26E+08
Product cost	€/kg	4,50E+01	4,50E+01	4,60E+01	4,60E+01	4,50E+01	4,50E+01	4,60E+01	4,60E+01
Raw Materials Cost	€/kg	5,32E+00	5,32E+00	6,09E+00	6,09E+00	5,32E+00	5,32E+00	6,09E+00	6,09E+00
Transport cost	€/year	1,67E+05	1,79E+05	3,18E+04	4,54E+04	1,67E+05	1,80E+05	3,19E+04	4,55E+04

3.5. Indicators aggregation

The main advantage of the methodology is that it allows comparison between different processes. Thus, we have compared the four different distribution network scenarios for both separation processes (DTSP and CDPSP).

A sustainability index was obtained by aggregating the results from the environmental, economic and social impact assessments. This process was performed in five different stages, as explained in the methodology chapter.

For the first stage, indicators prioritization and normalization, the indicators to be compared were selected:

- Environmental assessment: Human toxicity, freshwater aquatic ecotoxicity and terrestrial ecotoxicity

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- Social assessment: number of employees, number of women employed and number of fixed employers.
- Economic assessment: investment, microcapsules cost, raw materials cost and transport cost

Table 44 to Table 47 presents the indicators aggregation steps to obtain the sustainability index for the case study.

Table 44. Indicators results

			DTSP				CDPSP			
Area	**Indicator**	**Units**	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**
Environmental	**HTP**	Kg 1,4-DCB eq	8,32E+04	8,41E+04	2,77E+04	2,87E+04	8,07E+04	8,17E+04	2,52E+04	2,62E+04
	FAETP	Kg 1,4-DCB eq	1,31E+04	1,32E+04	2,35E+03	2,47E+03	1,29E+04	1,30E+04	2,19E+03	2,30E+03
	TAETP	Kg 1,4-DCB eq	1,15E+03	1,16E+03	5,42E+02	5,54E+02	1,10E+03	1,11E+03	4,91E+02	5,02E+02
Social	**# employees**	Quantity	1,76E+02	1,76E+02	1,18E+02	1,18E+02	1,76E+02	1,76E+02	1,18E+02	1,18E+02
	# women employed	Quantity	8,80E+01	8,80E+01	5,90E+01	5,90E+01	8,80E+01	8,80E+01	5,90E+01	5,90E+01
	# fixed employees	Quantity	6,60E+01	6,60E+01	4,40E+01	4,40E+01	6,60E+01	6,60E+01	4,40E+01	4,40E+01
Economical	**Investment**	€ total	2,25E+08	2,25E+08	2,26E+08	2,26E+08	2,25E+08	2,25E+08	2,26E+08	2,26E+08
	Microcapsules cost	€/kg	4,50E+01	4,50E+01	4,60E+01	4,60E+01	4,50E+01	4,50E+01	4,60E+01	4,60E+01
	Raw Materials Cost	€/kg	5,32E+00	5,32E+00	6,09E+00	6,09E+00	5,32E+00	5,32E+00	6,09E+00	6,09E+00
	Transport cost	€/year	1,67E+05	1,79E+05	3,18E+04	4,54E+04	1,67E+05	1,80E+05	3,19E+04	4,55E+04

Table 45. Indicators prioritization

		Environmental			Social			Economical			
		HTP	**FAETP**	**TAETP**	**# employees**	**# women employed**	**# fixed employees**	**Investment**	**Product cost**	**Raw Materials Cost**	**Transport cost**
DTSP	**Scenario 1**	0,19	0,21	0,17	0,15	0,15	0,15	0,12	0,12	0,12	0,20
	Scenario 2	0,19	0,21	0,18	0,15	0,15	0,15	0,12	0,12	0,12	0,21
	Scenario 3	0,06	0,04	0,08	0,10	0,10	0,10	0,13	0,13	0,13	0,04
	Scenario 4	0,07	0,04	0,08	0,10	0,10	0,10	0,13	0,13	0,13	0,05
CDPSP	**Scenario 1**	0,18	0,21	0,17	0,15	0,15	0,15	0,12	0,12	0,12	0,20
	Scenario 2	0,19	0,21	0,17	0,15	0,15	0,15	0,12	0,12	0,12	0,21
	Scenario 3	0,06	0,04	0,07	0,10	0,10	0,10	0,13	0,13	0,13	0,04
	Scenario 4	0,06	0,04	0,08	0,10	0,10	0,10	0,13	0,13	0,13	0,05
		1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00

As in case study 1, a comparison between indicators not together but per groups was made. In the environmental area, the same weight was given to FAETP and to TAETP due to the proximity and contact between the Medias. Same weights were given to these indicators than to the HTP, according to the weighting procedure of the Eco-indicator 99. In the social aspects, the same weigh was given to all indicators, since they were

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considered equally important. For the economic area, the same weigh was given to all indicators, since they are all measure in the same unit (€). Then, a comparison between the groups of indicators was made. The same weight was assigned to each group. So, a 0.33 was given to each one. It is important to note that the weights can vary according to the case study. After the calculations, the indicators prioritization was obtained. The weight per groups was multiplied by the weight per indicator to obtain the indicators prioritization (Table 46).

Table 46. Indicators weighting factors

Area	Indicator	Weight/group	Weight/indicator	Indicators Prioritization
Environmental	HTP	0,33	0,50	0,167
	FAETP	0,33	0,25	0,083
	TAETP	0,33	0,25	0,083
Social	# employees	0,33	0,33	0,111
	# women employed	0,33	0,33	0,111
	# fixed employees	0,33	0,33	0,111
Economical	Investment	0,33	0,25	0,083
	Microcapsules cost	0,33	0,25	0,083
	Raw Materials Cost	0,33	0,25	0,083
	Transport cost	0,33	0,25	0,083

Sustainability ranking results are shown on Table 47.

Table 47. Sustainability ranking

	Environmental			Social			Economical				
	HTP	**FAETP**	**TAETP**	**# employees**	**# women employed**	**# fixed employees**	**Investment**	**Product cost**	**Raw Materials Cost**	**Transport cost**	**Total**
Case 2 - Scenario 1	0,032	0,018	0,015	0,017	0,017	0,017	0,010	0,010	0,006	0,016	**0,16**
Case 2 - Scenario 2	0,032	0,018	0,015	0,017	0,017	0,017	0,010	0,010	0,006	0,018	**0,16**
Case 2 - Scenario 3	0,011	0,003	0,007	0,011	0,011	0,011	0,010	0,011	0,015	0,003	**0,09**
Case 2 - Scenario 4	0,011	0,003	0,007	0,011	0,011	0,011	0,010	0,011	0,015	0,004	**0,09**
Case 3 - Scenario 1	0,031	0,017	0,014	0,017	0,017	0,017	0,010	0,010	0,008	0,016	**0,16**
Case 3 - Scenario 2	0,031	0,018	0,014	0,017	0,017	0,017	0,010	0,010	0,008	0,018	**0,16**
Case 3 - Scenario 3	0,010	0,003	0,006	0,011	0,011	0,011	0,010	0,011	0,012	0,003	**0,09**
Case 3 - Scenario 4	0,010	0,003	0,006	0,011	0,011	0,011	0,010	0,011	0,012	0,004	**0,09**

From the sustainability ranking, it can be concluded that the decentralization of the production process and that train transportation options are the most sustainable ones.

Figure 42 presents a sustainability ranking comparison for the eight analysed cases.

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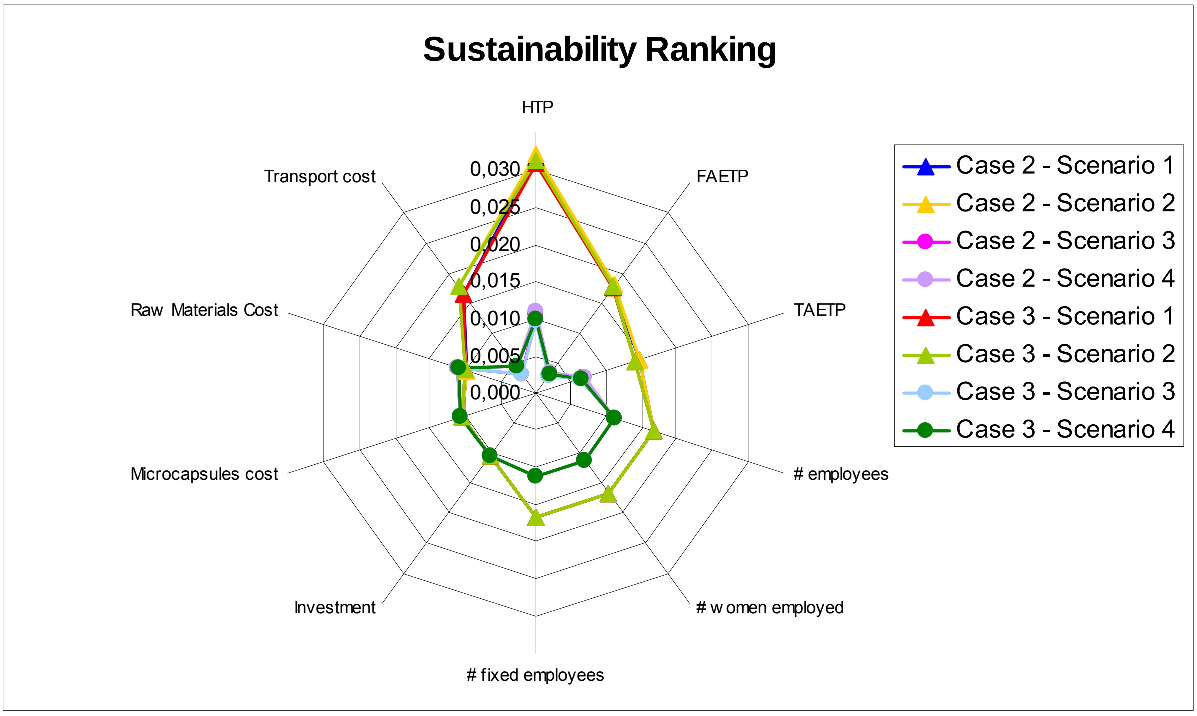

Figure 42. Triple bottom line framework

Figure 42 also shows that the decentralization of the production process is the more sustainable option.

4. Conclusions for Case Study 2

It was demonstrated that the SLCM methodology is a suitable tool for the sustainability evaluation of the case study, allowing the comparison of different transport types and distribution of production sites.

From the sustainability index calculation it can be concluded that decentralised production is more sustainable than centralised production, because of the reduction in the transport distances, considering that the transport from Madrid to the four distribution centres chosen is avoided when those centres are used to locate production.

Also the transport by train is more sustainable than the transport by trucks, because of the reduction of the cost and the environmental impacts related to the use of fuel.

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Chapter 6. Conclusions and Outlook

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Life Cycle Thinking is an efficient philosophy for process selection and decision-making. It is a data intensive method and requires considerable labour and cost. A methodological procedure for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology at design level named Sustainable Life Cycle Management (SLCM) methodology has been developed as an alternative to detailed life cycle analyze for process selection and decision-making. The SLCM encompasses environment, economic, and social aspects. A stepwise system of indexing has been proposed for each domain. These indices are combined to yield an overall index using a weighting procedure based on analytical hierarchy process (AHP). The weights in the analytical hierarchy process are determined by bibliography and expert opinion survey. In addition, the methodology includes: 1) definition of key indicators for eco-efficiency and sustainability assessment of industrial processes with multi-scale technology, and 2) a procedure for indicators selection, indicators calculation, normalization and weighting performing, sensitivity and uncertainty analysis and results communication.

A complete review on actual methodologies for sustainability evaluation, environmental, social and economical methods and indicators has been included within this work as a basis for the developed methodology.

The SLCM follows all the steps of the ISO 14040 series, analyzing the complete life cycle of the process to assess. It allows the analysis of the environmental, economic and social aspects and the potential impacts associated through all stages of the life cycle of the process analyzed (from cradle to grave). It uses indicators to analyze the impacts. It shows the individual results of each indicator. Impacts are calculated giving a set of selected indicators, which are agregated into an overall index. Results are graphically presented by means of a spiderplot diagram.

The SLCM can be used as a decision making tool for sustainability reporting since it integrates the three pillars of sustainability providing an objective criteria for decision making. It can be applied to any process with the same purpose, and it is clear and easy to follow. The application of the methodology is not time consuming and does not implied any supplementary costs. The presented SLCM methodology can be applied to any process or activity choosing in each case the corresponding set of inventory data and sustainability impact indicators.

The developed methodology has been translated to Microsoft® Excel® format, followed by a Matlab© programming in order to obtain the sustainability module for MICAP software developed by IMPULSE partners.

SLCM was proved on a case study included within the IMPULSE project. The case study has been defined via data collection and inventory performing for the environmental, social and economical points of view. Data for the inventory were collected from other IMPULSE partners, simulation tools such as MICAP and ASPEN, data obtained from bibliography, data estimated and approximated and the use of database information and proxies.

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Annexes

Annex 1. Existing Life Cycle Assessment methodologies

Next some of the existing methodologies will be explained.

(Dutch) Handbook on LCA or CML 2001

In 2001 CML (Center of Environmental Science of Leiden University) published a new "operational guide to the ISO standards". The (Dutch) Handbook on LCA provides a stepwise `cookbook' with operational guidelines for conducting an LCA study step-by-step, justified by a scientific background document, based on the ISO Standards for LCA. The different ISO elements and requirements are made operational to be `best available practice' for each step. The life cycle impact assessment methodology recommended is based on a midpoint approach covering all emission- and resource-related impacts, for which practical and acceptable characterization methods are available (Guinée et al., 2002). Best available characterization methods have been selected based on an extensive review of existing methodologies world-wide.

The CML Guide provides a list of impact assessment categories grouped into:
A: Obligatory impact categories (Category indicators used in most LCAs)
B: Additional impact categories (operational indicators exist, but are not often included in LCA studies)
C: Other impact categories (no operational indicators available, therefore impossible to include quantitatively in LCA)

For most impact categories a baseline and a number of alternative characterization methods is recommended and for these methods comprehensive lists of characterization and also normalization factors are supplied. Ecotoxicity and human toxicity are modelled adopting the multi-media USES-LCA model developed by Huijbregts (Huijbregts et al., 2000 and 2001). The Handbook provides characterization factors for more than 1500 different LCI-results.

Eco-indicator 99

Eco-Indicator 99 was developed in a top down fashion. The weighting was simplified by using three endpoints level, in ISO terminology: human health, ecosystem quality and resources. Another new idea in this method is the consistent management of subjective choices using the concept of cultural perspectives. This has lead to a good documentation of the choices and to the publication of three versions, each with a different set of choices. Other issues are the introduction of the DALY approach, the introduction of the PAF and PDF approach, as well as the surplus energy approach.

EDIP`97 & EDIP 2003

EDIP97 is a thoroughly documented midpoint approach covering most of the emission-related impacts, resource use and working environment impacts (Wenzel et al., 1997, Hauschild and Wenzel, 1998) with normalization based on person equivalents and weighting based on political reduction targets for environmental impacts and working environment impacts, and supply horizon for resources. Ecotoxicity and human toxicity are modelled using a simple key-property approach where the most important fate

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characteristics are included in a simple modular framework requiring relatively few substance data for calculation of characterization factors.

EDIP97 was updated through the EDIP2003 methodology (Hauschild and Potting, 2003) supporting spatially differentiated characterization modelling which covers a larger part of the environmental mechanism than EDIP97 and lies closer to a damage-oriented approach. This part of the general method development and consensus programme covers investigations of the possibilities for inclusion of exposure in the life cycle impact assessment of non-global impact categories (photochemical ozone formation, acidification, nutrient enrichment, ecotoxicity, human toxicity, noise).

EPS 2000d

The EPS 2000d is developed to be used for supporting choice between two product concepts. Category indicators are chosen for this purpose, i.e., they are suitable for assigning values to impact categories. Category indicators are chosen to represent actual environmental impacts on any or several of five safeguard subjects: human health, ecosystem production capacity, biodiversity, abiotic resources and recreational and cultural values. The characterization factor is the sum of a number of pathway-specific characterization factors describing the average change in category indicator units per unit of an emission, e.g. kg decrease of fish growth per kg emitted SO2. An estimate is made of the standard deviation in the characterization factors due to real variations depending on emission location etc. and model uncertainty. This means that characterization factors are only available, where there are known and likely effects. Characterization factors are given for emissions defined by their location, size and temporal occurrence. Most factors are for global conditions 1990 and represent average emission rates. This means that many toxic substances, which mostly are present in trace amounts, have a low average impact. Weighting factors for the category indicators are determined according to people's willingness to pay to avoid one category indicator unit of change in the safe guard subjects.

IMPACT 2002+

The IMPACT 2002+ life cycle impact assessment methodology proposes a feasible implementation of a combined midpoint/damage approach, linking all types of life cycle inventory results (elementary flows and other interventions) via 14 midpoint categories to four damage categories. For IMPACT 2002+ new concepts and methods have been developed, especially for the comparative assessment of human toxicity and eco-toxicity. Human Damage Factors are calculated for carcinogens and non-carcinogens, employing intake fractions, best estimates of dose-response slope factors, as well as severities. The transfer of contaminants into the human food is no more based on consumption surveys, but accounts for agricultural and livestock production levels. Indoor and outdoor air emissions can be compared and the intermittent character of rainfall is considered. Both human toxicity and ecotoxicity effect factors are based on mean responses rather than on conservative assumptions. Other midpoint categories are adapted from existing characterizing methods (Eco-indicator 99 and CML 2002). All midpoint scores are expressed in units of a reference substance and related to the four damage categories human health, ecosystem quality, climate change, and resources. Normalization can be performed either at midpoint or at damage level. The IMPACT

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2002+ method presently provides characterization factors for almost 1500 different LCI-results.

Swiss Ecoscarcity Method (Ecopoints)

The method of environmental scarcity - sometimes called Swiss Ecopoints method - allows a comparative weighting and aggregation of various environmental interventions by use of so-called eco-factors. The method supplies these weighting factors for different emissions into air, water and top-soil/groundwater as well as for the use of energy resources. The eco-factors are based on the annual actual flows (current flows) and on the annual flows considered as critical (critical flows) in a defined area (country or region).

The method has been developed top-down and is built on the assumption that a well established environmental policy framework (incl. the international treaties) may be used as reference framework for the optimization and improvement of individual products and processes. The various damages to human health and ecosystem quality are considered in the target setting process of the general environmental policy; this general environmental policy in turn is then the basis for the 'critical flows'. An implicit weighting takes place in accepting the various goals of the environmental policy. The ecopoints method contains common characterization/classification approaches (for climate change, ozone depletion, and acidification). Other interventions are assessed individually (e.g. various heavy metals) or as a group (e.g. NM-VOC, or pesticides).

The method is meant for standard environmental assessments, e.g., with specific products or processes. In addition, it is often used as an element of environmental management systems (EMS) of companies, where the assessment of the company's environmental aspects (ISO 14001) is supported by such a weighting method.

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Annex 2. Comparison between existing methodologies

Table 48 shows a comparison between the existing Life Cycle Assessment methodologies.

Table 48. Comparison between existing methodologies[12]

LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
Method description	Midpoint method with normalization	Damage approach, including Normalization and default Weighting sets	Midpoint method with normalization	Midpoint method with normalization	Category indicators at damage level + weighting as WTP to avoid damage	Midpoint+damage including normalization	Weighting method, based on environmental policy goals, to be used for midpoint categories and selected
Website Access Point	http://www.leidenuniv.nl/cml/ssp/projects/lca2/lca2.html	www.pre.nl/eco-indicator99/	http://ipt.dtu.dk/~mic/Projects.htm#EDIP97	http://ipt.dtu.dk/~mic/Projects.htm#EDIP2003	http://eps.esa.chalmers.se/	http://www.epfl.ch/impact	http://www.umweltschweiz.ch/buwal/eng/fachgebiete/fg_produkte/umsetzung/oekobilanzen/index.html
Reference	Guinée, J.B. (Ed.), M. Gorrée, R. Heijungs, G. Huppes, R. Kleijn, A. de Koning, L. van Oers, A. Wegener Sleeswijk, S.Suh, H.A. Udo de Haes, J.A. de Bruijn, R. van Duin and M.A.J. Huijbregts, 2002. Handbook on Life Cycle Assessment: Operational Guide to the ISO Standards. Kluwer Academic Publishers. Dordrecht	Goedkoop at al.(1999), check for updates at website (version April 2000)	Wenzel et al. (1997), Hauschild and Wenzel (1998)	Hauschild and Potting (2004), Potting and Hauschild (2004)	Steen (1999) and Steen(1999)	Jolliet et al.(2003)	Brand G., Braunschweig A., Scheidegger A., Schwank O.: Weighting in Ecobalances with the Ecoscarcity Method - Ecofactors 1997, BUWAL Series 297, 1998. German print available at the above web-adress; english PDF available at docu@buwal.admin.ch or for download at http://www.e2mc.com/BUWAL297%20english.pdf
Comments	Factors and updates downloadable on site	Three versions are published (Nierarchis, Individualist, Egalitarian. Below Hierarchist	Update available as EDIP2003 with site-dependent	Site-dependent characterization for European countries for	Factors and description downloadable on site	Factors and description downloadable on	Update for 2004 Swiss values in progress. The "Swiss ecopoints" are based on the

[12] Source: http://www.lci-network.de/cms/webdav/site/lca/shared/UNEP_SETAC%20LCIA%20corner/Summary%20of%20Methods_03_11_2004.pdf

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
		is described.	characterization for most non-global impact categories	most non-global impact categories		site	Swiss environmental policy; the method may be applied to other regions' environmental policy goals as well.
MIDPOINT CATEGORIES							
RELEASES							
Climate change	(42) kg CO2-eq./kg emitted M (GWP 100 as baseline; GWP 20, GWP 500, upper limit of net GWP and lower limit of net GWP as alternatives	(38) (DALYs/kg emission) M&D Damage model based on CO2, CH4 and N2) Representing substances with a lifetime of 100, 20 and 500 years. GWP equivalence factors for substances with similar lifetimes used to extend range of substances	(76 + factors for organics) kg CO2-eq./kg emitted M (GWP 100 as default, GWP 20 and GWP 500 as options) – includes factors for all organic substances of petrochemical origin	(76 + factors for organics) kg CO2-eq./kg emitted M (GWP 100 as default, GWP 20 and GWP 500 as options) – includes factors for all organic substances of petrochemical origin	(# factors) (units)	(38) kg CO2equ M (GWP 500) - kept as a separate damage category	(27) CO2-eq / kg emission (GWP 100) Global warming index based on 100 y time horizon, IPCC Second Assessment Report (IPCC 1996; direct climate forcing; with methane including indirect effects). GWP for additional emissions can be deducted from CFC-11
Stratospheric ozone depletion	(22) kg CFC-11-eq./kg emitted M (ODP infinite as baseline; ODP 5, 10, 15, 20, 25, 30 and 40 as alternatives)	(23) (DALYs/kg emission) M&D Damage model for CFCs, and ODP factors used to extrapolate to other substances (DALYs/kg emission)	(19) kg CFC-11-eq./kg emitted M (ODP, infinite)	(19) kg CFC-11-eq./kg emitted M (ODP infinite)	(*) (units)	(22) kg CFC-11 equ into air M&D (ODP infinite) Bqeq carbon-14 into air volume D M&D	(26) CFC-11-eq / kg emission Volumen
Human toxicity, including	(859)	(55) & (6)	(181)	(181)	(# factors)	(781)	(33)

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
workplace and indoor pollutants	kg 1,4-DCB-eq. emitted to air/kg emitted M Integrated multi-media fate, exposure and effect modelling based on USESLCA model of Huijbregts (infinite Toxicity Potentials (TPs) for global scale as baseline; global scale TPs for 20, 100 and 500 years time horizon and continental scale TPs for infinite time horizon as alternatives).	(DALYs/kg emission) M&D Fate and exposure calculated with EUSES, using a closed Europe setting (low wind speed, low water runoff). For metals some corrections are made in the air compartment. Also simple correction for population density differences for substances with short and long lifetime. Effect based on epidemiological studies collected by Hofstetter; damage, based on DALY method (without age weighting), using Murray et al. Fate and exposure based on empirical data collected by Hofstetter (1998); effect and damage based on epidemiological data and Daly calculation based on Murray et al.	m3 air/g emitted to air, water or soil; m3 water/g emitted to air, water or soil; m3 soil/g emitted to air, water or soil M Partial fate including transfer between compartments, photochemical oxidation and biodegradation, and human exposure. Effect based on human reference dose. Separate sub categories for human exposure through air, water, soil and groundwater). Working environment impacts from chemical exposure, noise and repetitive work	person M Site-dependent exposure factors for emissions to air to be used together with site generic EDIP97 characterisation factors for human toxicity via air to represent the extent to which the emission leads to human exposure. This is mainly for sensitivity analysis.	(units)	kg 1,4-DCB-eq. emitted to air/kg emitted kg chloroethylene into air equ into air (cancer & non cancer) kg PM2.5equ into air (respiratory inorg.) M&D Fate & exposure described by intake fraction (including intermittent rain and production based exposure) Effect factor based on best estimate (ED10: Effect-Dose 10%) and including illnesses severity. Human Damage Factor in DALY/kg emitted. Includes factors for respiratory effects and inside air emissions	g Various - no single "human tox"-category. Annual maxima for emission (e.g. particles to air, heavy metals to air, water and top soil, pesticides to ground water), based on the various considerations in defining legal concentration or flow limits into air, water and top soil.
Ionising radiation	(49) yr.kBq-1; Sv.m3.Bq-1.yr-1 D	(25) (DALYs/kg emission)	-	-		(25) Bqeq carbon-14 into air volume D M&D	(2) Volumen

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
	(Frischknecht et al., 2000 damage factors as baseline; Solberg-Johansen, 1998 screening factors level I and II as alternatives)	Fate, exposure, effect and damage based on Frischknecht et al., 1999, relying much on Dreicer et al 1995 for fate and exposure of routine emissions from French nuclear fuel cycle. Damage step includes rough estimates for hereditary effects	-	-		like ecoindicator 99	Volume of radioactive waste (as long-term potential for ionising radiation)
Non-ionising radiation	-	-	-	-	-	-	-
Accidents	(XX) (units) M (Unweighted aggregation of victims)		-	-	-	(XX) (units) M&D Cases and DALY from statistics can be added to other human health impacts	-
Photo oxidant formation	(126) kg ethylene-eq./kg emitted; kg formed ozone/kg emitted M (High NOx POCP as baseline; MIR, MOIR, EBIR and low NOx POCP as alternatives)	(50) (DALYs/kg emission) M Eco-indicator 99 name: Respiratory organic, POCP values used to calculate Ozone formation. Ozone treated as respiratory inorganic impact category (see above)	(82 individual substances and 13 VOC mixtures) kg ethylene-eq./kg emitted M (POCP, high or low Background concentration of NOx) Regression expressions for calculation of missing characterisation factors based on kOH	(All NMVOCs, and CH4, Nox and CO) m2 ecosystem*ppm*hours/g emitted; pers*ppm*hours/g emitted M (but close to damage - exposure above threshold times duration) Separate site-dependent modelling of exposure of vegetation and of human beings in two separate sub categories		(130) kg ethylene equ into air M&D (POCP)	"NM-VOC" & NOx g NM-VOC Emission maxima for NMVOC and NOx according to the national Air Hygiene goals
Noise	(*) (Pa^2.s) (Unweighted aggregation of sound in Pa2.s)	(0) (DALYs/Pa^2.s) Applied experimentally in line with Mueller Wenk 2003, but not included in methodology report	-	- pers*sec Noise from traffic in Potting and Hauschild (2004)	-	- (units) (Compatible with Mueller - Wenk, 2003)	- (An earlier version of the Swiss Eco-points included a provisional noise assessment)

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
Acidification	(4) kg SO2-eq. in Switzerland/kg emitted; kg SO2-eq./kg emitted M (Average AP expressed in SO2 equivalents based on RAINS model as baseline; generic H+ release based AP and RAINS based region (site) dependent AP as alternatives)	(3) (PDF/m3/yr) Acifdification and Eutrophication are combined. Direct link between emissions and damage. ONLY airborne emissions: Fate using Dutch SMART model, Effect, using Dutch MOVE model. Calculates PDF/m3/yr directly using Ellenberg curves. Waterborne emissions not included!	(12) kg SO2-eq. /kg emitted M (AP based on SO2)	(12) m2 unprotected ecosystem/g emitted; M (but close to damage - area of ecosystem exposed above critical load)		(10) kg SO2 equ into air M for aquatic, M&D for terrestrial (AP based on SO2)	(3 resp. 5) H+ moles-e / kg emission AP based on SO2 for HF, HCl; NH3 & NOx are covered based on more stringent goals
Eutrophication	(12) kg PO43--eq./kg emitted; kg NOx-eq. in Switzerland/kg Emitted M (Average EP expressed in PO4 equivalents based on the Redfield ratio as baseline; average European EP based on RAINS model and RAINS based region (site) dependent EP as alternatives)	(3) (DALYs/ke emission) See acidification	(12) kg NO3--eq./kg emitted; kg Neq/ kg emitted; kg P-eq/kg emitted M (N and P equivalents, aggregation possible based on Redfield factor (NO3—equivalents))	(12) m2 unprotected ecosystem/g emitted; M Separate modeling of Aquatic eutrophication (exposure factor to be combined with the EDIP97 site-generic characterization factor) and terrestrial eutrophication (area of ecosystem exposed above critical load).		(10) kg PO43- equ into water M for aquatic M&D for terrestrial (P equivalent based on Redfield factor, by default P-limited only)	(4) g N and g P P: annual emission limit into swiss lakes; N: annual emission limits into sweet water (in view of receiving sea basins)
Ecotoxicity (Fate, exposure and effect	(892)	(200)	(192)	(192)		(393) aquatic ecotox, (393) terrestrial ecotox	(42)

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
should at least be considered)	kg 1,4-DCB-eq. emitted to fresh water, sea water or industrial soil/kg emitted M Integrated multi media fate, exposure and effect modelling based on USESLCA model of Huijbregts (infinite Toxicity Potentials (TPs) for global scale as baseline; global scale TPs for 20, 100 and 500 years time horizon and continental scale TPs for infinite time horizon as alternatives; separate TPs for fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity and terrestrial ecotoxicity).	(PDF/m3/yr)/kg emission Fate calculated with EUSES, using a closed Europe setting (low wind speed, low water runoff). For metals some corrections are made in the air compartment. PAF method used to determine Potentially Affected fraction assuming effect addition and assuming background PAF. Conversion from PAF to PDF using conversion factor 10. Correction for pesticides; the impact on agricultural soil is set to zero, as this effect is also covered in land use	m3 water/g emitted to air, water or soil; m3 soil/g emitted to air, water or soil M Partial fate including transfer between compartments, photochemical oxidation and biodegradation. Effect based on PNEC	m3 water/g emitted to air, water or soil; m3 soil/g emitted to air, water or soil M Exposure factors for emissions to water and soil to be used together with site generic EDIP97 characterisation factors for ecotoxicity in these compartments to represent the extent to which the emission leads to human exposure. Mainly for sensitivity analysis		kg triethylene glycol equ into water / soil M&D AMI method: Assessment of mean impacts based on HC50 (geometric mean of EC50), Affected & Disappeared fraction of species	g Various - no single "eco tox"-category. Annual maxima for emission (e.g. acids to air, heavy metals to air, water and top soil, oxygen consuming carbon to surface waters, pesticides to ground water), based on the various considerations in defining legal concentration or flow limits into air, water and top soil.
RESOURCE USE							
Land use & habitat losses	- m2.yr	(15)	-	-		(15) m2 organic arable crop	(4) volume and weight of controlled waste deposition (use of scarce space fit for specific waste depositions)

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
	Unweighted aggregation of land competition	Based on Köllner 1999, but with some changes. Köllner collected data for species richness in Swiss lowlands per land use type. Uses the Species area relationship; also to include regional aspect. Regional impact. Both occupation and conversion, but conversion uses simple default restoration time of 30 years. Problem. Species data for agricultural area's probably too low, as Edges of croplands are not fully included				Adoption of Eco-indicator 99 method	(1 for all)
Energy extractions	(98) (Primary energy carriers and minerals assessed together. ADP based on ultimate reserves and extraction rates as baseline; economic reserves and extraction rates, ultimate or economic reserve only, and energy content as alternatives)	(9) (units) Fossil fuels: surplus energy concept further developed for fossil.	(xx) Weighting based on supply horizon	-		(9) MJ total Cumulative non renewable primary energy demand	input of energy (=consumption of exergy), expressed as energy content of consumed energy carriers (fossile, nuclear, hydro, etc.) see below -
Mineral extractions	-	(12) (units)	(xx)	-	-	(20) MJ surplus	-

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
		Minerals: Surplus energy concept of Mueller Wenk applied, but implemented in a somewhat different way	Weighting based on supply horizon			Additional cumulative non renewable primary energy demand to close life cycle	
Water resource use	-	-	(xx) Weighting based on supply horizon (for non-sustainable use)	-	-	(1) MJ Cumulative primary energy demand in inventory	-
Soil quality	-	-	(xx) Weighting based on supply horizon (for non-sustainable use)	-	-	-	-
Biotic resource use	For biotic resources no baseline; reserves and bioaccumulation rate as alternative	-	-	-	-	-	-
DAMAGE ASSESSMENT CATEGORIES							
Human Health							
Human health		(1) (DALYs) Human Health includes mortality and morbidity			(169) (pyears) Includes as damages subcategories, (158) YOLLyears of lost life, (161) severe morbidity , (1) severe nuisance and (7) nuisance	(4) midpoint categories brought together (DALYs) Human Health includes mortality and morbidity	
DAMAGE ASSESSMENT CATEGORIES							
Biotic and Abiotic Natural Environment							
Biotic Natural Environment		(1) (PDF/m2/yr)/kg emission Ecosystem Quality			(160) Unitless NEX, normalized extinction of species, dimensionless	(4) midpoint categories brought together PDF-m2-year Ecosystem Quality	

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LCIA Methodology	(Dutch) LCA Handbook or CML 2001	Eco-indicator 99	EDIP97	EDIP2003	EPS 2000d	IMPACT 2002(+)	(SWISS) ECOSCARCITY
Abiotic Natural Environment						kg CO2 equ Climate change kept as separate damage on life support system	
Abiotic and Biotic Natural Resources							
Abiotic Natural Resources	(98) (units) Primary energy carriers and minerals assessed together. ADP based on ultimate reserves and extraction rates as baseline; economic reserves and extraction rates, ultimate or economic reserve only, and energy content as alternatives	-			(81) kg / kg reserves (1) Fossil oil, (1) fossil coal, (1) fossil natural gas and (78?) element reserves		(3) MJ (1) Fossil oil, (1) fossil coal, (1) fossil natural gas
		(1) MJ / MJ surplus Resources (MJ surplus energy)			(2) kg Drinking water and Irrigation water, (characterization factor of 1, as the flow mostly is determined directly in the LCI. The same is relevant for the 81 abiotic resources)	(2) midpoint categories brought together MJ primary non ren. energy Natural resources	
					(7) mole H+ equivalents Base cat-ion capacity of soil		
Biotic Natural Resources					-112	Biotic natural resources as a	

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LCIA Methodology	**(Dutch) LCA Handbook or CML 2001**	**Eco-indicator 99**	**EDIP97**	**EDIP2003**	**EPS 2000d**	**IMPACT 2002(+)**	**(SWISS) ECOSCARCITY**
					kg / kg reserves (112) crop production, (112) wood production, (9) fish & meat production		
Abiotic and Biotic Man-Made Environment							
Abiotic Man-Made Environment					Recreational and cultural values		
Biotic Man-Made Environment					also see biotic natural resources above + defined adhoc categories	Biotic natural resources as a proxy	

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Annex 3. Impact categories related to Groups A, B and C of the CML 2001 methodology

A. Obligatory or Baseline Impact Categories

Group A, "Obligatory or Baseline impact categories", comprises categories covered in most LCA studies. This themes are mandatory for any LCA study.

- <u>Depletion of abiotic resources</u>

"Abiotic resources" are natural resources (including energy resources) such as iron ore, crude oil and wind energy, which are regarded as non-living.

- <u>Impacts of land use</u>

This category covers a range of consequences of human land use. A distinction has been made between use of land with impacts on the resources aspects and use of land with impacts on biodiversity, life support functions, etc.

  - *Land competition*

This subcategory of land use impacts is concerned with the loss of land as a resource, in the sense of being temporarily unavailable.

- <u>Climate change</u>

Climate change is defined as the impact of human emissions on the radioactive forcing (i.e. heat radiation absorption) of the atmosphere. This may in turn have adverse impacts on ecosystem health, human health and material welfare. Most of these emissions enhance radiative forcing, causing the temperature at the earth's surface to rise. This is popularly referred to as the "greenhouse effect".

- <u>Stratospheric ozone depletion</u>

Stratospheric ozone depletion refers to the thinning of the stratospheric ozone layer as a result of anthropogenic emissions. This causes a greater fraction of solar UV-B radiation to reach the earth's surface, with potentially harmful impacts on human health, animal health, terrestrial and aquatic ecosystems, biochemical cycles and materials.

- <u>Human Toxicity</u>

This impact category covers the impacts on human health of toxic substances present in the environment.

- <u>Ecotoxicity</u>

This impact category covers the impacts of toxic substances on aquatic, terrestrial and sediment ecosystems.

  - *Freshwater aquatic ecotoxicity*

Freshwater aquatic ecotoxicity refers to the impacts of toxic substances on freshwater aquatic ecosystems.

  - *Marine aquatic ecotoxicity*

This impact category covers impacts of toxic substances on marine aquatic ecosystems.

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- *Terrestrial ecotoxicity*

Terrestrial ecotoxicity refers to impacts of toxic substances on terrestrial ecosystems.

- Photo-oxidant formation

Photo-oxidant formation is the formation of reactive chemical compounds such as ozone by the action of sunlight on certain primary air pollutants. These reactive compounds may be injurious to human health and ecosystems and may also damage crops.

- Acidification

Acidifying pollutants have a wide variety of impacts on soil, groundwater, surface waters, biological organisms, ecosystems and material (buildings).

- Eutrophication

Eutrophication covers all potential impacts of excessively high environmental levels of macronutrients, the most importants are nitrogen (N) and phosphorus (P). Nutrient enrichment may cause an undesirable shift in species composition and elevated biomass production in both aquatic and terrestrial ecosystems. In addition, high nutrient concentrations may also render surface waters unacceptable as a source of drinking water. In aquatic ecosystems increased biomass production may lead to a depressed oxygen level, because of the additional consumption of oxygen in biomass decomposition (measured as BOD, biological oxygen demand). As emissions of degradable organic matter have a similar impact, such emissions are also treated under the impact category "eutrophication".

B. Study-specific Impact Categories

Group B, "Study-specific impact categories", comprises categories that may merit inclusion, depending on the goal and scope of the LCA study and whether appropriate data are available.

- Impacts of land use

The category "Impacts of land use" covers a range of consequences of human land use. A distinction has been made between use of land with impacts on the resources aspects and use of land with impacts on biodiversity, life support functions, etc.

- Loss of life support function

In this impact category, the problems defined are the effects on life support functions resulting from interventions such as harvesting biotic resources, or the destruction or alteration of land.

- Loss of biodiversity

In this impact category, the problems defined are the effects on biodiversity resulting from interventions such as harvesting biotic resources, or the destruction or alteration of land.

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- Ecotoxicity

This impact category covers the impacts of toxic substances on aquatic, terrestrial and sediment ecosystems. The area of protection is the natural environment (and natural resources).

  - *Freshwater Sediment ecotoxicity*

Freshwater sediment ecotoxicity refers to impacts of toxic substances on the sediment of freshwater ecosystems.

  - *Marine Sediment ecotoxicity*

Marine sediment ecotoxicity refers to impacts of toxic substances on the sediment of sea ecosystems.

- Impacts of ionizing radiation

The impact category "impacts of ionizing radiation" covers the impacts arising from releases of radioactive substances as well as direct exposure to radiation, in building materials for example. Exposure to ionizing radiation is harmful to both human beings and animals. The areas of protection are therefore human health, the natural environment and natural resources.

- Odour

Odour becomes a problem when a given concentration of odorous substances is experienced as pleasant. Whether an odour is experienced as stench will depend on the particular individual exposed. Above a certain emission level, however, every individual will experience it as such. The area of protection is human health.

- Malodorous air

This subcategory involves airborne odour.

- Noise

Noise, or noise nuisance, refers to the environmental impacts of sound. In principle, these impacts could cover at least human health and ecosystem health, but the environmental mechanisms are complex, non-linear and highly dependent upon local circumstances. Moreover, noise is similar to odor in that a given level of exposure is experienced differently by different individuals. Something considered a nuisance by one person might be appreciated by another, as exemplified by the case of loud music. Hence, whether or not sound waves will lead to "nuisance" depends partly on the actual situation and partly on the person interviewed.

- Waste heat

Emissions of waste heat may increase temperatures on a local scale: in a city or lake, for example. They cannot contribute to global warming on a scale such as that associated with emissions of greenhouse gases. The effects on ecosystems of waste heat emissions to the air are negligible. Depending on local conditions, the discharge of waste heat into surface waters may result in a substantial temperature rise, with a consequent impact on local aquatic ecosystems. The areas of protection are the natural environment and natural resources.

- Casualties

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This impact category refers to casualties resulting from accidents. The area of protection is human health.

C. Other Impact Categories

Group C, "Other impact categories", comprises several categories for which alternative characterization methods may be available.

- Depletion of biotic resources

"Biotic resources" are material resources (including energy resources) regarded as living, e.g. rainforest, elephants. Depending an the precise definition adopted, this impact category has only natural resources, or natural resources, human health and the natural and man-made environment as areas of protection.

- Desiccation

Desiccation refers to a group of related environmental problems caused by water shortages due to groundwater extraction for industrial and potable water supply, enhanced drainage and water management (i.e. manipulation of the water table). This may lead to lowered water table, reduced seepage, introduction of water from other areas and (consequently) changes in natural vegetation. The area of protection is the natural environment.

- Odour

Odour becomes a problem when a given concentration of odorous substances is experienced as pleasant. Whether an odor is experienced as stench will depend on the particular individual exposed. Above a certain emission level, however, every individual will experience it as such. The area of protection is human health.

- Malodorous water

This subcategory deals with water-borne odour.

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Annex 4. Formulas to Calculate Environmental Profile within CML 2001 methodology

Table 49. Formulas to calculate the environmental profile

Impact Categories	Characterization equation	Unit of indicator result
- Depletion of abiotic resources	$\sum_i ADP_i \times m_i$ ADP_i= Abiotic depletion potential of resource *i* m_i= quantity of resource *i* used	kg (Sb eq.) Sb= Antimony
- Impacts of land use		
▪ Land competition	$a \times t \times 1$ *a*= area used *t*= occupation time	m^2.yr
- Climate change	$\sum_i WGP_{a,i} \times m_i$ $WGP_{a,i}$= Global warming potential for substance *i* integrated over a years m_i= quantity of substance *i* emitted	kg (CO_2 eq.) CO_2= Carbon dioxide
- Stratospheric ozone depletion	$\sum_i ODP_{\infty,i} \times m_i$ $ODP_{\infty,i}$= stedy-state Ozone depletion potential for substance *i* m_i= quantity of substance *i* emitted	kg (CFC-11 eq.) CFC-11 = trichlorofluoromethane
- Human Toxicity	$\sum_i \sum_{ecom} HTP_{ecom,i} \times m_{ecom,i}$ $HTP_{ecom,i}$= human toxicity potential (characterization factor) for substance *i* emitted to emission compartment *ecom* (=air, fresh water, seawater, agricultural soil or industrial soil) $m_{ecom,i}$= emission of substance *i* to medium *ecom*	kg (1,4-DCB eq.) 1,4-DCB = 1,4-dichlorobenzene
- Ecotoxicity		
▪ Freshwater aquatic ecotoxicity	$\sum_i \sum_{ecom} FAETP_{ecom,i} \times m_{ecom,i}$ $FAETP_{ecom,i}$= Freshwater aquatic ecotoxicity potential (characterization factor) for substance *i* emitted to emission compartment *ecom* (=air, fresh water, seawater, agricultural soil or industrial soil) $m_{ecom,i}$= emission of substance *i* to medium *ecom*	kg (1,4-DCB eq.) 1,4-DCB = 1,4-dichlorobenzene
▪ Marine aquatic ecotoxicity	$\sum_i \sum_{ecom} MAETP_{ecom,i} \times m_{ecom,i}$ $MAETP_{ecom,i}$= Marine aquatic ecotoxicity potential (characterization factor) for substance *i* emitted to emission compartment *ecom* (=air, fresh water, seawater, agricultural soil or industrial soil) $m_{ecom,i}$= emission of substance *i* to medium *ecom*	kg (1,4-DCB eq.) 1,4-DCB = 1,4-dichlorobenzene

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▪ Terrestrial ecotoxicity	$\sum_i \sum_{ecom} TETP_{ecom,i} \times m_{ecom,i}$ $TETP_{ecom,i}$= Terrestrial ecotoxicity potential (characterization factor) for substance *i* emitted to emission compartment *ecom* (=air, fresh water, seawater, agricultural soil or industrial soil) $m_{ecom,i}$= emission of substance *i* to medium *ecom*	kg (1,4-DCB eq.) 1,4-DCB = 1,4-dichlorobenzene
- Photo-oxidant formation	$\sum_i POCP_i \times m_i$ $POCP_i$= Photochemical ozone creation potential for substance *i* m_i= quantity of substance *i* emitted	kg (C_2H_4 eq.) C_2H_4= Ethylene
- Acidification	$\sum_i AP_i \times m_i$ AP_i= Acidification potential for substance *i* emitted to the air m_i= emission of substance *i* to the air	kg (SO_2 eq.) SO_2= Sulfur dioxide
- Eutrophication	$\sum_i EP_i \times m_i$ EP_i= Eutrophication potential for substance *i* emitted to the air, water or soil m_i= emission of substance *i* to the air, water or soil	kg (PO_4^{3-} eq.) PO_4^{3-} = phosphate

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Annex 5. Calculation Method for Inherent Safety Index (ISI)

To calculate ISI, scores for seven parameters (inventory, flammability, explosiveness, toxicity, temperature, pressure and yield) are shown in Table 50, Table 51, Table 52, Table 53, Table 54, Table 55, and Table 56 (Heikkilä, 1999).

Table 50. Inventory scores

Inventory (Tonnes)	***Score***
0.1-250	1
251-2500	2
2501-7000	3
7001-16000	4
16001-26000	5
26001-38000	6
38001-50000	7
50001-65000	8
65001-80000	9
80001-100000	10

Table 51. Flammability scores

Flammability	***Score***
Non-combustible	0
FP>140°F	1
100°F<FP<140°F	2
FP<100°F BP>100°F	3
FP<100°F BP<100°F	4
FP = Flash point BP = Boiling point	

Table 52. Explosiveness scores

Explosiveness S = (UEL – LEL)%	***Score***
$0 \leq S < 10$	1
$10 \leq S < 20$	2
$20 \leq S < 30$	3
$30 \leq S < 40$	4
$40 \leq S < 50$	5
$50 \leq S < 60$	6
$60 \leq S < 70$	7
$70 \leq S < 80$	8
$80 \leq S < 90$	9
$90 \leq S < 100$	10

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Table 53. Toxicity scores

Toxicity (ppm)	*Score*
TLV < 0.001	8
0.001 ≤ TLV < 0.01	7
0.01 ≤ TLV < 0.1	6
0.1 ≤ TLV < 1.0	5
1.0 ≤ TLV < 10.0	4
10.0 ≤ TLV < 100.0	3
100.0 ≤ TLV < 1000.0	2
1000.0 ≤ TLV < 10000.0	1
1.0% ≤ TLV	0

Table 54. Temperature scores

Temperature (°C)	**Score**
T < -25	10
-25 ≤ T < -10	3
-10 ≤ T < 10	1
10 ≤ T < 30	0
30 ≤ T < 100	1
100 ≤ T < 200	2
200 ≤ T < 300	3
…	…
700 ≤ T < 800	8
800 ≤ T < 900	9
900 ≤ T	10

Table 55. Pressure scores

Pressure (psi)	*Score*	
0 – 90	1	
91 – 140	2	
141 – 250	3	
251 – 420	4	
421 – 700	5	
701 – 1400	6	
1401 – 3400	7	
3401 – 4800	8	
4801 – 6000	9	
6001 – 8000	10	+ 1 point per 2500 psi

Table 56. Yield scores

% yield	*Score*
100	0
90 – 99	1
80 – 89	2
70 – 79	3
60 – 69	4
50 – 59	5
40 – 49	6
30 – 39	7
20 – 29	8

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10 – 19	9
0 –10	10

Each reaction step in the route is given a score, which is the sum of two parts, the chemical and process scores for the step.

The **Chemical Score** is for the properties of the chemicals involved in the step that is inventory, flammability, explosiveness and toxicity. The scores for the four parameters are summed for each chemical species present. The highest of these sums becomes the chemical score for that step. **The Process Score** is for the reaction conditions that are temperature, pressure and yield. The scores for these are summed to give the process score for the step. The total for the step is the sum of the chemical and the process scores. The index is calculated by summing the scores obtained for each reaction step in the route.