

## SUSTAINABLE INNOVATION OF CHEMICALS: USING LCA AS A METRICS IN ADVANCING AND SCALING UP GREEN CHEMISTRY RESEARCH

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*Keywords: Sustainable innovation, chemicals, LCA metrics, green chemistry*

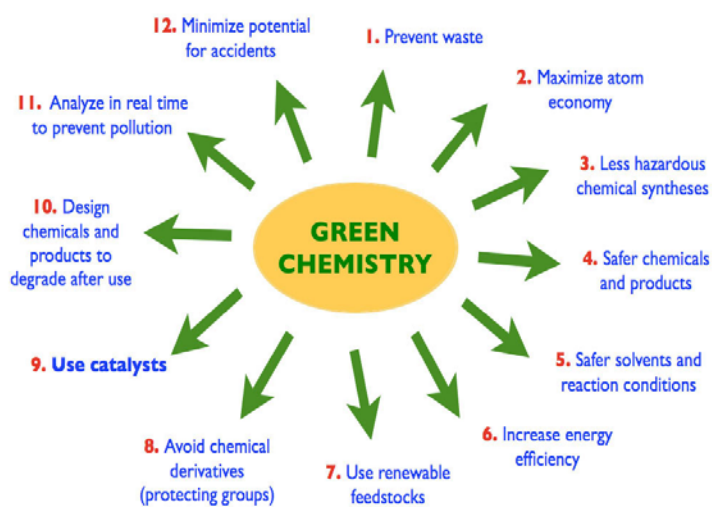
### ABSTRACT

The concept of Green Chemistry was coined in the 1990s and can be briefly defined as applying the pollution prevention approach to chemistry. LCA is a technique to assess environmental impacts associated with all the stages of a product's life from-cradle-to-grave. If this method is applied in the form of a gate-to-gate LCA it provides the environmental profile, or footprint, of a chemical or material composed of multiple chemicals. A criticism to the 12 green chemistry principles as a tool is their qualitative nature. Using two examples, this paper shows how LCA can help evaluating the 12 principles in concrete cases of advancing green chemistry research towards the sustainable innovation of chemicals. Emphasis is made to show the potential for using LCA as a metrics in scaling up this research.

### INTRODUCTION – GREEN CHEMISTRY (GC)

The concept of Green Chemistry (GC) was coined by US EPA in the 1990s and can be briefly defined as applying the pollution prevention approach to chemistry (Anastas and Warner, 1998). Overall the concept has a strong focus on reducing and eliminating the use and generation of hazardous substances. In order to make this concept operational, the USEPA developed the Twelve Principles of Green Chemistry; see Figure 1.

These principles constitute the backbone of GC and a universal code of practice for the eco-design of



Anastas and Warner (1998)

Figure 1. The Twelve Principles of Green Chemistry

chemicals and chemical processes (Clark and Macquarrie, 2002). A criticism to the 12 principles of Green Chemistry as a tool is that some of them have qualitative nature, which can lead to difficulties when the progress made by introducing GC practices has to be measured, or when trade-offs between principles arise (Muñoz, 2012).

## METHODS – LIFE CYCLE ASSESSMENT (LCA)

The scientific community noticed this limitation of Green Chemistry, and several methods for environmental assessment in GC have been proposed. Life Cycle Assessment has been highlighted as a suitable tool in this context by several authors such as Anastas and Lankey (2000), Domenech et al (2002), Gustafsson and Börjesson (2007) and Muñoz (2012).

According to the ISO 14040 series Life Cycle Assessment is a technique to assess environmental impacts associated with all the stages of a product's life from-cradle-to-grave. It allows accounting for the resource consumption and emissions at each step of the product life cycle. If this method is applied in the form of a gate-to-gate LCA it provides the environmental profile, or footprint, of a chemical or material composed of multiple chemicals.

## RESULTS – USING LCA AS A METRICS FOR TWO GC EXAMPLES

Life Cycle Assessment is applied in two cases to demonstrate how it can be used as a metrics to quantify the results achieved on the basis of the green chemistry principles. One example is the case of two chemical reactions to produce maleic anhydride and the other is the production of hydrogen from fossil fuels or from vegetable oils.

### *Maleic anhydride*

Domenech et al (2002) present an example with two routes of obtaining maleic anhydride that are compared using LCA, to ascertain which one is the environmentally more sustainable one. A possible way to produce maleic anhydride is the oxidation of benzene with oxygen gas over a  $V_2O_5$  catalyst, at 3 to 5 bar of pressure and at a temperature of 350 to 450 °C. The use of butene as feedstock is an alternative way of obtaining produce maleic. Figure 2 presents chemical reactions, the thermodynamic conditions and the Atom Economy (AE) of the two reactions. Table 1 explains which Green Chemistry principles have been applied.

Figure 3 presents the Life Cycle Impact Assessment results from the LCA for the comparison of these two routes of obtaining maleic anhydride. The results clearly demonstrate how LCA allows communicating with quantitative sustainability information the application of the qualitative Green Chemistry principles.

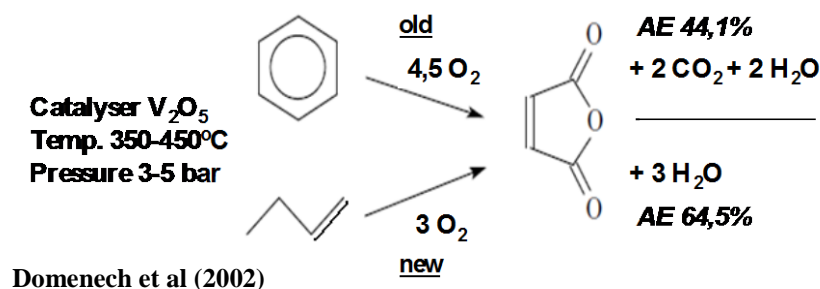


Figure 2. Two routes of obtaining maleic anhydride (AE – Atom Economy)

Green Chemistry Principle	Industrial Motivation
Atom Economy	$\Delta$ AE 20,4%
Simple and safe process	Easy recovery and separation due to reduced by-products
Less waste and emission	Emissions of CO <sub>2</sub> avoided
Minimisation of toxicity	Toxicity of benzene avoided <b>Cavani et al (2009)</b>

Table 1. The application of the Green Chemistry principles and the industrial motivation

System	GWP g CO <sub>2</sub>	AP. g SO <sub>x</sub>	EP. g PO <sub>4</sub> <sup>3-</sup>	ODP g C <sub>2</sub> H <sub>2</sub>	Solid waste g	Energy Cons. MJ
<b>Production of 1 mole maleic anhydride from benzene</b>						
Benzene prod.	42	0.60	0.069	0.26	0.76	5.8
Oxygen prod.	31	0.33	0.008	N	N	0.28
Waste Treat.	88	0,0012	N	N	0.36	0.06
Energy prod.	-67	-0.31	N	N	N	-0.49
<b>TOTAL</b>	<b>94</b>	<b>0.63</b>	<b>0.077</b>	<b>0.26</b>	<b>1.1</b>	<b>5.65</b>
<b>Production of 1 mole maleic anhydride from butylene</b>						
Benzene prod.	28	0.41	0.044	0.16	0.46	3.8
Oxygen prod.	20	0.22	0.006	N	N	0.19
Waste Treat.	0,0010	0.018	0.001	N	0.54	0.09
Energy prod.	-40.5	-0.19	N	N	N	-0.30
<b>TOTAL</b>	<b>7.5</b>	<b>0.46</b>	<b>0.051</b>	<b>0.16</b>	<b>1.0</b>	<b>3.78</b>

**GWP** – Global Warming Potential  
**AP** – Acidification Potential  
**EP**- Eutrophication Potential  
**ODP** – Ozone Depletion Potential  
**Cons.** – Consumption  
**Prod.** - Production

**Domenech et al (2002)**

Figure 3. Life Cycle Impact Assessment results for the routes of producing maleic anhydride

### Hydrogen

Following the GC principle to use renewable feedstock Marquovich et al (2002) studied pathways to produce hydrogen from vegetable oils. A life cycle inventory was prepared to assess the CO<sub>2</sub> (fossil) emissions and then to calculate the Global Warming Potential (GWP), associated to the production of hydrogen by the steam reforming of hydrocarbon feedstocks (methane and naphtha) and vegetable oils (rapeseed oil, soybean oil and palm oil).

Results show that the GWPs associated with the production of hydrogen by steam reforming in a 100 years time frame are 9.71 and 9.46 kg CO<sub>2</sub>-equivalent/kg H<sub>2</sub> for natural gas and naphtha, respectively. For vegetable oils, the GWP decreases to 6.42 kg CO<sub>2</sub>-equivalent/kg H<sub>2</sub> for rapeseed oil, 4.32 for palm oil and 3.30 for soybean oil. A dominance analysis determined that the part of the process that has the largest effect on the GWP for vegetable oil-based systems is harvesting and oil production. The quantitative information provided by LCA allows choosing the vegetable oil with the lowest carbon footprint. Applying only the GC principle does not provide this level of detail to orientate further research.

## DISCUSSION – ADVANCING AND SCALING UP GC RESERACH

The two simple examples put into evidence that using LCA is useful to advance Green Chemistry research since it facilitates the choice of the most environmentally sustainable path forward and provides a consistent basis for a professional communication about relevant sustainability characteristics like carbon footprint. Applying the Green Chemistry principles and quantifying the progress in sustainable innovation of chemicals made by LCA offer a decent framework for moving towards a sustainable chemistry.



The 6th International Conference on Life Cycle Management in Gothenburg 2013

LCA is of particular interest when getting out of the chemistry lab into an industrial scale. Then resource efficiency and cost consideration become the crucial criteria for moving ahead in the innovation process or discarding an originally promising new chemical reaction or process. However, precaution needs to be applied in interpreting LCA results from lab experimentation. It does not mean that the idea for a novel technology is not good; it just means it is not resource-efficient yet but with maturation the production processes may still get through a continuous learning period to an unexpected level of efficiency.

## CONCLUSIONS AND PERSPECTIVES

A criticism to the 12 principles of Green Chemistry as a tool is their qualitative nature, which can lead to difficulties when the progress made by introducing GC practices has to be measured, or when trade-offs between principles arise. The scientific community noticed this limitation, and several methods for environmental assessment in GC have been proposed. LCA has been highlighted as a suitable tool in this context by many authors.

Using only two literature examples, this paper shows how LCA can help evaluating the 12 GC principles in concrete cases of advancing green chemistry research towards the sustainable innovation of chemicals. A particular strength of LCA is the role it can play as a metrics in insuring resource efficiency when scaling up Green Chemistry research. Evidently, precautions should be taken in interpreting LCA results from lab-scale chemical experiments.

Further work foreseen implies to integrate the existing GC metrics like effective mass yield and atom economy in an indicator framework with Life Cycle Impact Assessment and to apply LCA to green synthesis pathways like use of microwave, ultrasound or ionic liquids.

## ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support of the Institute of Molecular Sciences (ISM) and the Region of Aquitaine, France, for allowing the corresponding author and his colleagues to carry out this research and to present our work at the conference.

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