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Process Analysis Using *Umberto Carbon Footprint* Tool

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Abstract

The software Umberto Carbon Footprint calculates CO_2 footprint of products or activities. It is based on analysis of primary and secondary footprints during the product lifecycle. It uses the ecoinvent database to analyse individual contribution of the resources consumption required for the footprint of the final product.

Umberto Carbon Footprint was applied to two processes where the streams and resources were characterized using the process simulator Aspen Plus: A) production of cumene from benzene and B) production of acetone from IPA (Isopropyl alcohol). The analysis was carried out for each process at two different scenarios (with and without simplified energetic integration).The results show an improvement on the carbon footprint value for the scenarios with energetic integration and a good agreement with ecoinvent database values

Umberto Carbon Footprint was also applied at one Portuguese chemical company to a formaldehyde process (patent Perstorp Formox®). Real industrial data was used on the streams and resources characterization. The carbon footprint obtained for F-100 (maximum production system scenario) shows a relative deviation of 1.8% comparing to ecoinvent database value.

Keywords: Modeling, Carbon Footprint, Umberto software, Industrial Process.

1. Introduction

Carbon footprint is a relative measurement of the amount of CO_2 release on the environment during the life cycle of a product or activity. Normally it's calculated from the analyses of direct and indirect emissions of resources consumed on a certain process. All streams of the industrial process must be previously characterized by a process simulation or using the industrial data. This tool could help in the discussion of different operating conditions scenarios, such as raw material diversity, process integration degree, utilities type, among others.

Nowadays this issues is has become increasingly important, and big supermarkets chains in UK and USA were wondering about putting the CO_2 footprint on the products descriptions labels, granting to the consumer the option of a more responsible choice in terms of ecologic matter.

The methodologies for carbon footprint calculations are still growing and it is emerging as an important tool for sustainability analysis. The concept of carbon footprinting has permeated and is being commercialized in all the areas of life and economy, but there is little coherence in definitions and calculations of carbon footprints among the studies. Carbon footprint is intended to be a tool to guide the relevant emission cuts and verifications, its standardization at international level are therefore necessary. Pandey et al. (2011) made a review where they describe the prevailing carbon footprinting

methods and raise the related issues. Some studies are being made as calculation of the corporate carbon footprint of the cement industry by MC3 methodology by Cagiao, et al. (2011). Yuttitham, et al., (2011) determined the carbon footprint of sugar produced from sugarcane in eastern Thailand. Graphical representation of carbon footprint reduction for chemical processes was applied by Tjan et al. (2010).
In this paper the carbon footprint calculation and analysis of chemical products with the application of software Umberto for Carbon Footprint using simulation and real industrial data.

2. Process simulator approach

2.1. Cumene process
Cumene is produced from a reaction in gas phase between benzene and polypropylene, with a main reaction (1) and parasite one (2):

$$\text{Propylene} + \text{Benzene} \longrightarrow \text{Cumene} \quad (1)$$

$$\text{Propylene} + \text{Cumene} \rightarrow \text{P} - \text{diisopropil benzene} \quad (2)$$

It was considered a minimum annual production of 120 kton of cumene with a specification of 99% in molar purity without any kind of heat integration (Scenario 1).

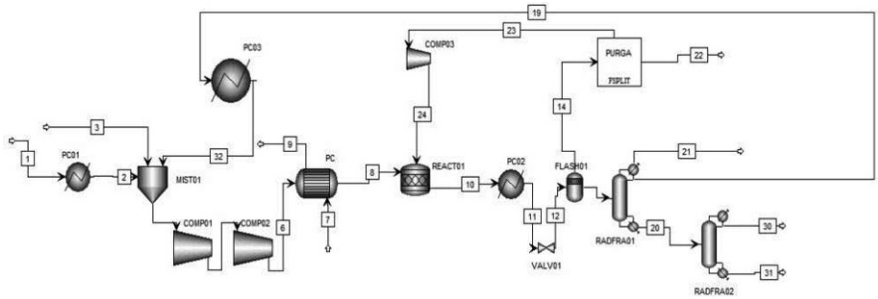

Figure 1: Cumene Process diagram in AspenPlus®. (Scenario 1)

An alternative diagram was tested with a simple energy integration of reactor effluent as hot fluid on exchanger named PC (Scenario 2).The hot utility used in Figure through stream 7 was removed.

Table 1: CO_2 Footprint and main contributions for the cumene process

Carbon Footprint (kg CO2 eq.)	
Scenario 1	Scenario 2
3.74	3.48

Contributions for the footprint			
Scenario 1		Scenario 2	
Benzene	65%	Benzene	70%
Propylene/ Propane	21%	Propylene/ Propane	22%
Others	14%	Others	8%

As expected it was noted an improvement of the CO_2 footprint of the process with simple energy integration that corresponds to a decreasing of 7% of the CO_2 footprint. The contribution of field “Others” (table 2) was smaller in the integrated process because this field includes the consumption of energetic resources that were reduced with the energetic integration.

2.2. Acetone process

The process of production of acetone from IPA contains a main reaction (3) and 2 other parasite ones (4) and (5).

$$\text{Isopropanol} \rightarrow \text{Acetone} + \text{Hydrogen} \quad (3)$$

$$\text{Isopropanol} \rightarrow \text{Propylene} + \text{water} \quad (4)$$

$$\text{Propylene} + \text{Hydrogen} \rightarrow \text{Propane} \quad (5)$$

It was considered a minimum annual production of 120 kton of acetone with a specification of 99% in molar purity (Scenario 1).

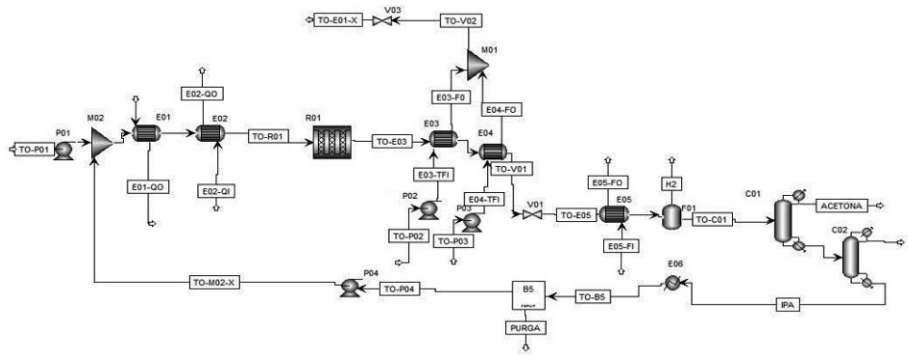

Figure 2: Acetone process diagram in AspenPlus®. (Scenario 1)

Also an alternative scenario was tested with simple energy integration. It was produced steam on the exchangers E03 and E04 and was recirculated to E01 (Scenario 2).

Table 2: CO_2 Footprint and main contributions for the acetone process

Carbon Footprint (kg CO_2 eq.)	
Scenario 1	Scenario 2
3.11	2.95

Contributions for the Footprint			
Scenario 1		Scenario 2	
IPA	77%	IPA	81%
Net steam	14%	Net steam	15%
Others	9%	Others	4%

The result is analogous of the previous process. It was verified a footprint decreasing of 5%.

3. Chemical Plant Data aproach

The carbon footprint calculation using the software Umberto for Carbon footprint is also applied to a real chemical plant data, instead of the previous approach where data was obtained by simulation with a process simulator.

This approach was applied to a process of production of formaldehyde type Perstorp Formox® of a Portuguese chemical industry. The formaldehyde production occurs on a fixed bed reactor through the partial oxidation of methanol.

The main reaction is strongly exothermic, and the heat of reaction is used to produce steam in exchanger E-2/1. The units E-18, E-22 and E-15/1 constitute the emission control system (ECS) which control the gas emissions to the atmosphere.

The equipment and streams before T-1 and T-2 are double and work in parallel, system-1 (S-1) and system-2 (S-2). The main product (F-50) is collected in T-2 and the Product F-30 on T-1.

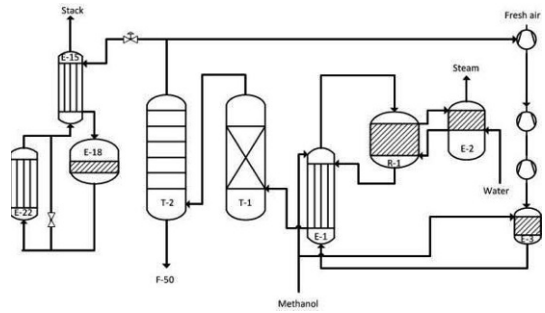

Figure 3: Simplified formaldehyde process diagram based on the Industrial site analysed.

Several production scenarios were tested:

- Scenario **3500-0**: Minimum production status, S-1 with a fresh methanol consumption of 3500 kg/h and S-2 stopped with only F-100.
- Scenario **0-4900** : S-2 with a fresh methanol consumption of 4900 kg/h and S-1 stopped;
- Scenario **3500-3500 :** S-1 with a fresh methanol consumption of 3500 kg/h and S-2 with a fresh methanol consumption of 3500 kg/h;
- Scenario **4900-4600:** S-1 with a fresh methanol consumption of 4900 kg/h and S-2 with a fresh methanol consumption of 4600 kg/h.

The scenarios with higher productions rates are the ones with smaller footprint. The carbon footprint is analysed by kg of product produced and is strongly dependent of the raw-materials utilization, and consequently in terms of process efficiency, so is expectable smaller footprints for those scenarios because they are the most efficient ones (also in observed in economical terms).

Table 3: CO_2 footprint of formaldehyde process – F100 and F-30

Methanol Consumption				
Scenario	S-1 (kg/h)	S-2 (kg/h)	CO_2 footprint (kg CO_2 eq.) F-100	CO_2 footprint (kg CO_2 eq.) F-30
3500-0	3500	0	1.11	-
0-4900	0	4900	1.22	9.91
3500-3500	3500	3500	1.07	13.45
4900-4600	4900	4600	1.09	16.49

It is predicted by ecoinvent 2.2 a carbon footprint for a formaldehyde process type Perstorp Formox® of 1.11 kg CO2 eq., for a maximum production system. Comparing this one with the value for scenario 4900-4600 is observed a relative deviation of 1.8%. The cause of deviation is explained by some differences in the calculation by ecoinvent and this one:

- Input values in ecoivent are from literature and project predicted values of several European production units.

- The ecoinvent footprint considers the contribution of final product transportation and in this project the formaldehyde was for own consumption.
- Ecoivent value uses input values from another process patent (silver catalysis) in addition to the patent Perstorp Formox®.
- Contribution of catalyst for the footprint is higher in ecoinvent because of a more regular replacement is used on the units analyzed.

Table 4: Individual contributions of Carbon footprint : F-100 and F-30

Contributions for the footprint								
Scenario	**3500-0**		**0-4900**		**3500-3500**		**4900-4600**	
	F-100	F-30	F-100	F-30	F-100	F-30	F-100	F-30
Methanol	73.3%	-	78.8%	78.9%	82.7%	83.2%	84.7%	84.5%
Electricity	3.5%	-	5.0%	4.3%	5.2%	4.2%	5.6%	6.0%
Chemical plant infrastructure	8.3%	-	6.1%	6.9%	5.2%	5.1%	3.4%	3.9%
Stack emissions	13.3%	-	9.1%	9.6%	6.9%	7.2%	5.1%	5.4%
Others	1.5%	-	1.1%	0.3%	0.1%	0.3%	1.2%	0.3%

Other causes of deviation lies on some approximations used in the footprint calculations as the assumption of CO_2 stack emissions similar for all scenarios tested and on the estimation of cooling water flows. In the future a deeper analysis will be done to overcome some practical difficulties encountered.

4. Conclusions

The Umberto for Carbon Footprint allows two different approaches for calculation of chemical processes footprints. With auxiliary data obtained for instance in a process simulator or plant data, the software becomes very easy and quick to use. The results obtained in this work show a good agreement with the ones from ecoinvent data base. In the future this contribution could be integrated with SustainPro® tool (Carvalho et al., 2008) to provide a more reliable sustainability analysis. It seems to be also an important tool to compare different process design scenarios.

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