PASI

Pan-American Advanced Studies Institute

Tutorial 3: Modeling and Dynamic Simulation with EMSO

Life Cycle Assessment Tool Integrated to EMSO

Simone Miyoshi*, Argimiro R. Secchi
*smiyoshi@peq.coppe.ufrj.br

Introduction

Low Carbon Economy

- **Minimization** of greenhouse gas (GHG) **emissions** for industrial processing and power generation
- **Design** and **Simulation** of production process with **lower** carbon footprint.

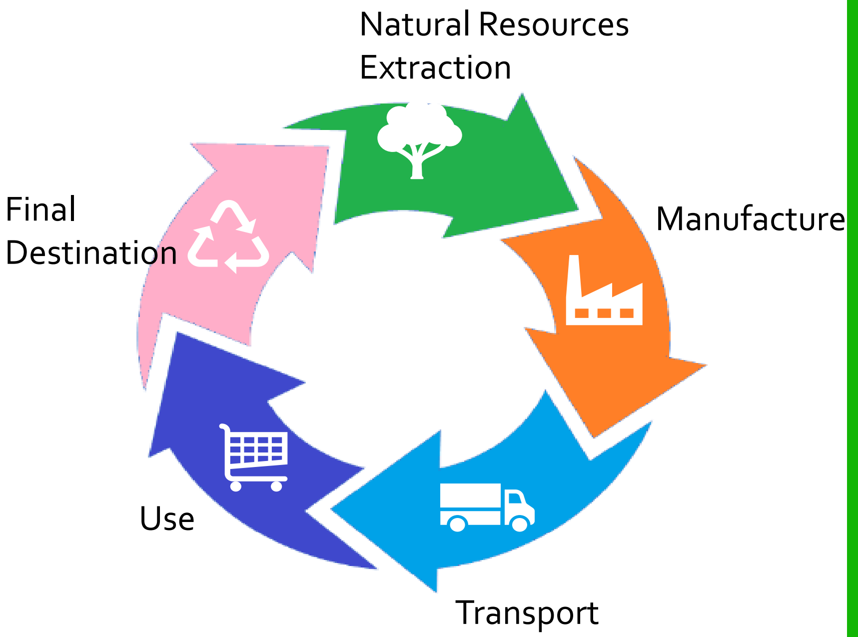
Need of **integrated** **Life Cycle Assessment** tools for **Process Simulation, Design** and **Optimization**.

Introduction

Life Cycle Assessment:

LCA is defined by the ISO 14040 as the compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle.

Definitions of environmental metric to process evaluation.



Introduction

- ✓ **Government Policy**
- ✓ **Decision-making Process**
- ✓ **Demonstrate** the process is **Green**
- ✓ Product **Marketing**

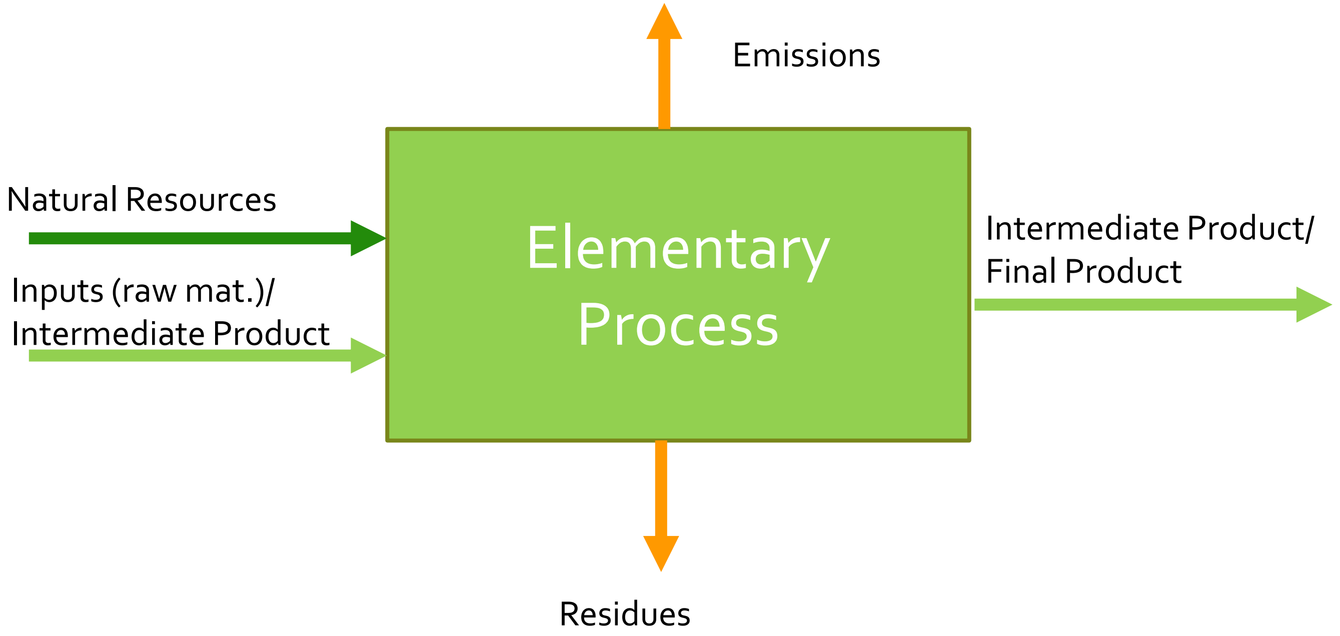
Introduction

Life Cycle Assessment

Goal and Scope	• Goal (application, purpose, intended audience) • Assumptions (Functional Unit, System boundaries, Allocation procedures, quality requirements)
Life Cycle Inventory	• Data collection (Inputs / Outputs) • Validation
Impact Assessment	• Selection of Assessment Methods • Selection of Assessment Categories • Classification and Characterization
Interpretation	• Identification of significant issues • Evaluation • Conclusions and recommendations

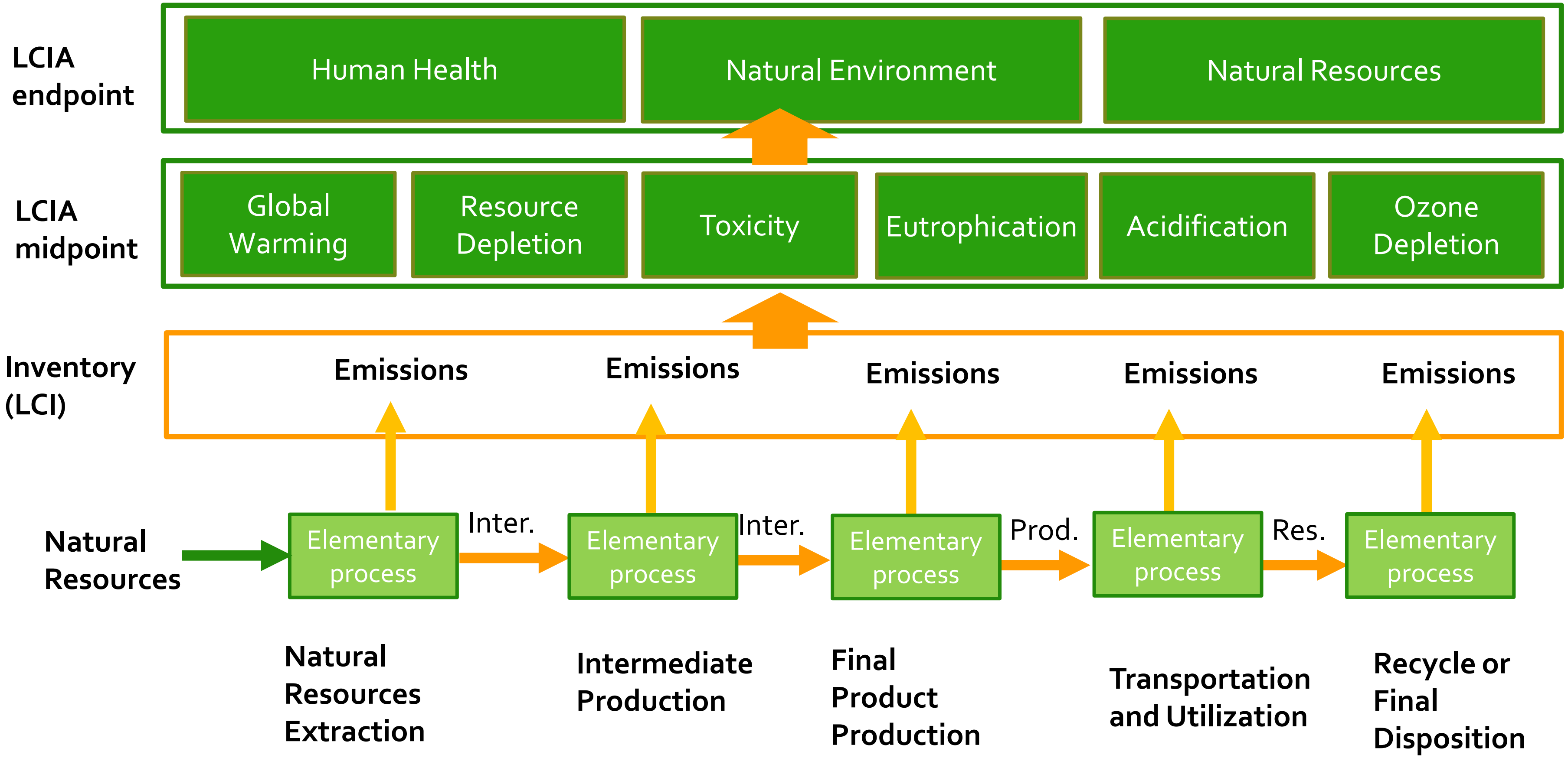
Introduction

Life Cycle Assessment Concepts
Elementary Process



Introduction

Life Cycle Assessment



Introduction

Some Life Cycle Assessment Categories

Category	Impact e Effects	Main Substances	Unity
Global Warming Potential (GWP 100 Years)	Climate Change, extreme climate events	CO_2, N_2O, CH_4	kg CO_2-eq
Ozone Layer Depletion Potential (ODP)	Increase of UV rays intensity, skin cancer	Trichlorofluoromethane (CFC-11), Halon 1301, Halon 1211	kg CFC-11 –eq
Eutrophication Potential (EP)	Emission of macronutrients such as nitrogen (N) and phosphorus (P) and carbon (C) into the environment: Algal blooms, oxygen depletion	NH_3, P, PO_4, NO_3	kg PO_4-eq
Acidification Potential (AP)	Damage to vegetation, rivers and lakes; material damage	SO_x, NH_3, NO_x	kg SO_2-eq
Photochemical oxidation Potential (POCP)	Damage to human health and ecosystems and can also damage agricultural crops	VOC, CO, NO_x	kg C_2H_4 eq
Human Toxicity Potential (HTP)	Acute and chronic toxicity to humans	Benzene, Cupper, Lead	kg 1,4-DB eq (1,4-dichlor-benzene)
EcoToxicity	Acute and chronic toxicity in ecosystems	1,4-dichlorobenzene, Mercury, Arsenic	kg 1,4-DB eq (1,4-dichlor-benzene)

Introduction

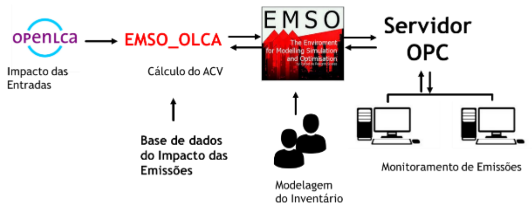
EMSO:

- **Free** for Academic use
- **Equation-Oriented** Simulator
- **Easy** to create new models: **Flexibility**
- **Fast:** lower computational time
- **Interface** with **Python**, C++, Matlab, Scilab, OPC, Excel, LibreOffice

OpenLCA:

- **Free, OpenSource**
- Several LCIA databases: **EcoInvent**, **Agri-footprint**,...
- **Atualization** of the impact assessment databases

EMSO_OLCA



Characteristics

- ✓ Flexibility
- ✓ Computational Speed (LCA of ethanol): 0.296 s
- ✓ Accuracy (LCA of ethanol): mean error of 0.0015%
- ✓ Integrated to **functionalities** of **EMSO**
- ✓ **Emissions impact** is accessed by **OpenLCA database**

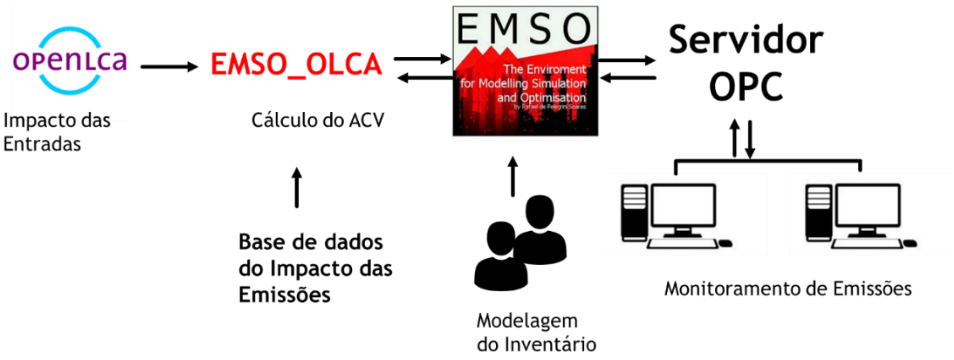
- ✓ **OpenLCA Impact Methodologies Available**:
  - ✓ 99 methodologies: IPCC, 2013; CML, 2001; ReCiPe, 2016; ...
  - ✓ 1479 Characterization Factors

- ✓ **OpenLCA** database update

EMSO_OLCA

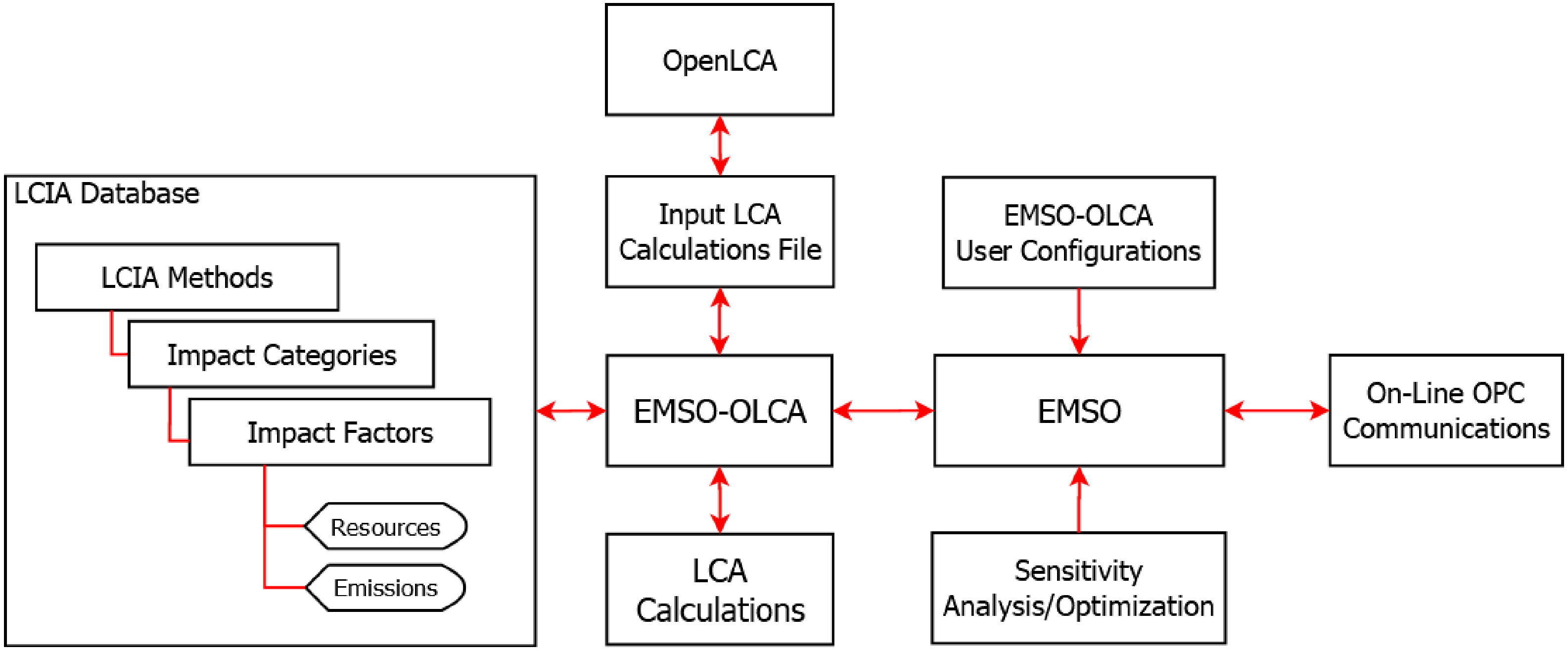
Applications:

- ✓ Identification of **bottom necks** and improvement opportunities
- ✓ Chemical Process **Routes** Selection
- ✓ **Process design** decisions: Eg. Different equipment configurations, process variables values
- ✓ Process **Monitoring**
- ✓ Process **Control**



EMSO_OLCA

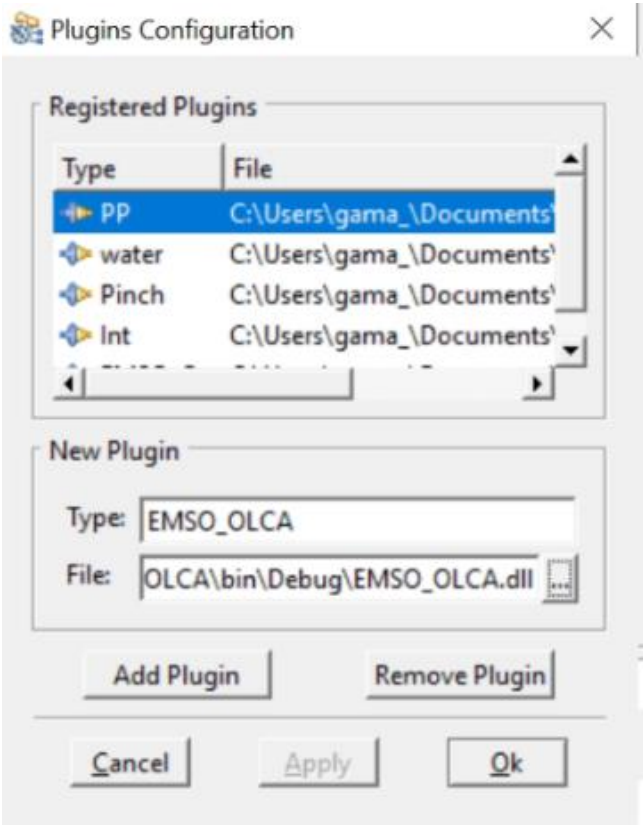
EMSO_OLCA Framework



EMSO_OLCA

Installation

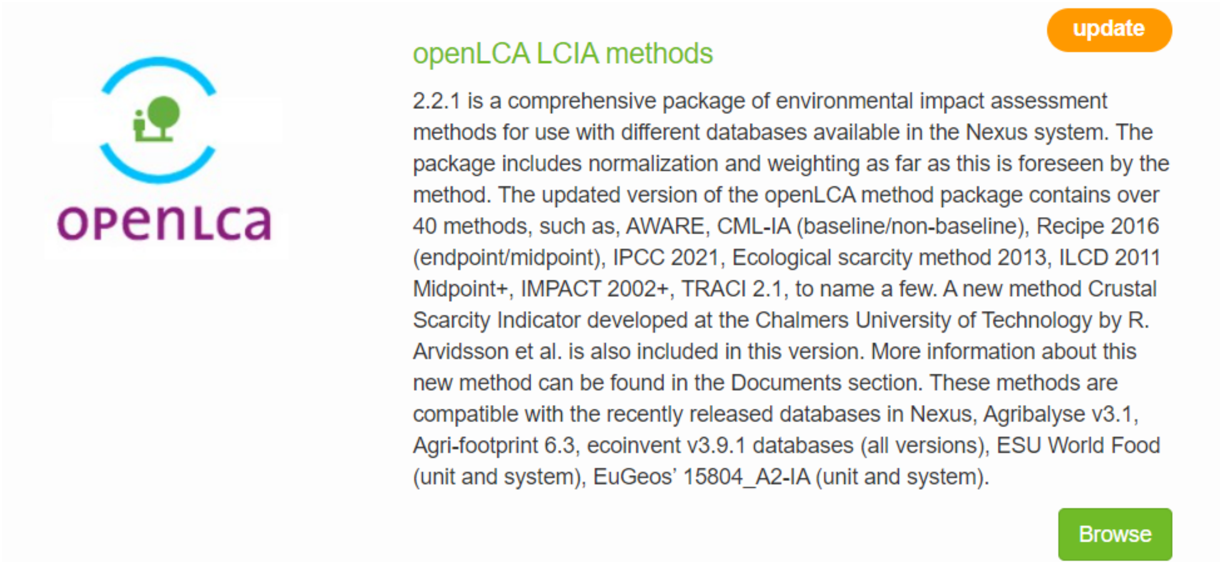
- ✓ For installation, the file EMSO_OLCA library should be informed on EMSO in Menu> Config>Plugins
- ✓ In the field New Plugin:
  - ✓ Type: EMSO_OLCA
  - ✓ File: Path to library



EMSO_OLCA

LCIA Database

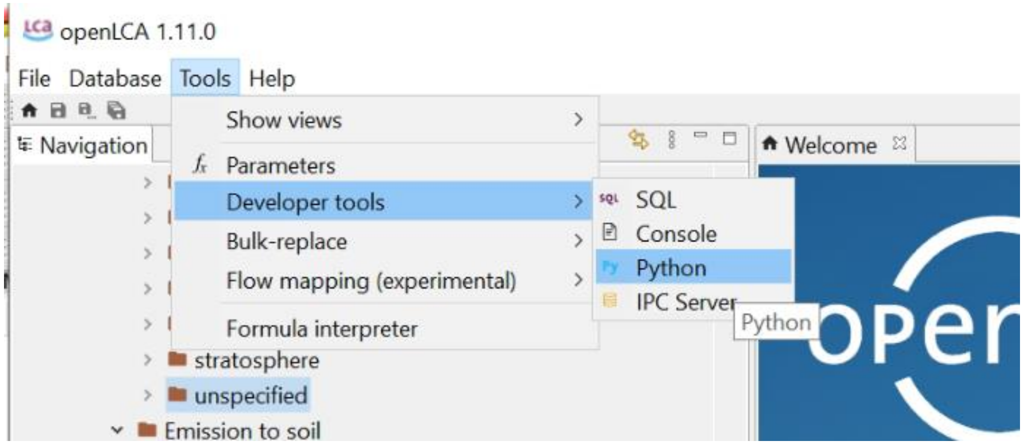
- ✓ Database is available on the NEXUS-OPENLCA website (***nexus.openlca.org/databases***). It can be downloaded for free (OpenLCA LCIA methods)
- ✓ The integration format with EMSO-OLCA is **JSON-LD**
- ✓ Note that the methodology should be compatible with the LCI
- ✓ ***DataBasePath*** will be the path to this folder.



EMSO_OLCA

Input LCA File

EMSO-OLCA entries are imported directly from OpenLCA and their impact is calculated through Menu TOOLS > Developer Tools > Python.



EMSO_OLCA

Input LCA File

To export the entries in a .csv file, please:

- ✓ Run the code in Python
- ✓ Select the entries to be considered
- ✓ Select the Life Cycle Assessment method
- ✓ Indicate the location to save the .csv file with the results of input impacts.

EMSO_OLCA

Elementary Flows

Elementary flows are defined as natural resources, emissions or waste. These must be configured according to the type (emission to air, water, soil or resource or waste or immaterial emission) and according to the location, as stated in the OpenLCA definitions.

For example (see OpenLCA),

ElementaryFlowPath1: Emission to air

ElementaryFlowPath2: high population density/low population density/ unspecified/stratosphere/lower stratosphere + upper troposphere

ElementaryFlowPath1: Emission to water

ElementaryFlowPath2: fóssil-/fresh water/ground water/lake/ocean/ river/ surface water/unspecified

EMSO_OLCA

EMSO_OLCA User Configurations Syntax

PARAMETERS

```
obj    as Plugin (Type= "EMSO_OLCA",
DataBasePath=[“C:/Users/usuario/Documents/EMSO_OLCA/methods_database”],
MethodName= ["MethodName"],
ImpactCategory=["ImpactCategory1", " ImpactCategory2"],
InputFileName=[“C:/Users/usuario/Documents/EMSO_OLCA/export_input.csv”],
Inputs=["name of input1", "name of input 2"],
OutputName=["name of the output 1"],
OutputUnit=["kg"],
ElementaryFlows=["Emission1","Emission2",“ResourceName1","ResourceName"],
ElementaryFlowPath1=["Emission to air", “Emission to air”, “Resource”,”Resource”],
ElementaryFlowPath2=["low population density","low population density","in water",
"land"],
UnitFileName=["C:/Users/usuario/Documents/EMSO_OLCA/EMSO_OLCA_units.csv"],
MethodologyType=["attributional"], # ou “consequential”
AllocationType=["mass"]); # ou “energy” ou “economic”
```

EMSO_OLCA

LCA Calculations

$$LCIA_c = \sum_i IF_{c,i} \times LCI_i$$

(Jolliet et al., 2010)

$$f_k = \frac{par_k \cdot m_k}{\sum_j \left(par_j \cdot m_j\right)}$$

(Guinée, 1995)

EMSO_OLCA

EMSO_OLCA Basic LCAModel Syntax

```
Model LCABasic
    PARAMETERS
outer NoComps as Integer;
outer obj as Plugin(Type="EMSO_OLCA");

    ni as Integer (Brief="Number of Inputs", Default=2);
    ncf as Integer (Brief="Number of Characterization Factors", Default=3);
    no as Integer (Brief= "Number of Outputs", Default=2);
    ne as Integer (Brief= "Number of ElementaryFlows (emissions+resources)", Default=2);
    nc as Integer (Brief= "Number of Consequential Input", Default=0);
    alloc_par(no) as Real (Default=1, Lower=1e-5);


    VARIABLES

    cf(ncf, ni) as Real;
    ef(ncf, ne) as Real;
    r (ncf, no) as Real;
    p (ncf, ni+ne+nc) as Real;

    input_values(ni) as Real (Default=1);
    emission_values(ne) as Real(Default=1);
    output_values(no) as Real (Default=1, Lower=1e-5);

    EQUATIONS

    [ef(1,:),ef(2,:),ef(3,:),ef(4,:),ef(5,:),ef(6,:),ef(7,:),ef(8,:),ef(9,:),ef(10,:),ef(11,:)] = obj.EmissionFactor();

    [cf(1,:),cf(2,:),cf(3,:),cf(4,:),cf(5,:),cf(6,:),cf(7,:),cf(8,:),cf(9,:),cf(10,:),cf(11,:)]  = obj.CharacterizationFacto

    # keep input values and emissions values in kg
    [r(1,:), r(2,:), r(3,:), r(4,:), r(5,:), r(6,:), r(7,:), r(8,:), r(9,:), r(10,:), r(11,:)] =
                                obj.LcaCalc(input_values, emission_values, output_values, alloc_par);

    [p(1,:), p(2,:), p(3,:), p(4,:), p(5,:), p(6,:), p(7,:), p(8,:), p(9,:), p(10,:), p(11,:)] =
                                obj.LcaPercentual(input_values, emission_values, output_values, alloc_par);

end
```

Case Study Syntax

```
CaseStudy CogenerationLowPCondEle as LCA_cogeracao_baixa_cond
VARY
wE103.Q=[-50:-50:-300]*'MW';
RESPONSE
greet.bagasse;
water;
vapor;
OPTIONS
Dynamic = false;
GuessFile = "F18_cond.rlt";
NLASolver(File = "sundials",
            RelativeAccuracy = 1e-3,
            AbsoluteAccuracy = 1e-6,
            MaxIterations = 100        );
end
```

EMSO_OLCA Test

Ethanol Test Case

EcoInvent 3.8, ethanol production autonomous plant, BR, 1Kg

Impact category	Reference unit	OpenLCA Result	EMSO Result	% Error
Abiotic depletion	kg Sb eq	$4.2916 \cdot 10^{-6}$	$4.2962 \cdot 10^{-6}$	0.1083%
Abiotic depletion (fossil fuels)	MJ	3.2862	3.2862	-0.0001%
Acidification	kg SO2 eq	$1.3946 \cdot 10^{-2}$	$1.3946 \cdot 10^{-2}$	0.0001%
Eutrophication	kg PO4--- eq	$7.4082 \cdot 10^{-3}$	$7.4082 \cdot 10^{-3}$	-0.0001%
Fresh water aquatic ecotox.	kg 1,4-DB eq	$1.3882 \cdot 10^{-1}$	$1.3882 \cdot 10^{-1}$	0.0000%
Global warming (GWP100a)	kg CO2 eq	$6.5146 \cdot 10^{-2}$	$6.5140 \cdot 10^{-2}$	-0.0090%
Human toxicity	kg 1,4-DB eq	$2.5019 \cdot 10^{-1}$	$2.5019 \cdot 10^{-1}$	-0.0001%
Marine aquatic ecotoxicity	kg 1,4-DB eq	$2.5725 \cdot 10^{+2}$	$2.5726 \cdot 10^{+2}$	0.0000%
Ozone layer depletion (ODP)	kg CFC-11 eq	$1.9625 \cdot 10^{-8}$	$1.9639 \cdot 10^{-8}$	0.0686%
Photochemical oxidation	kg C2H4 eq	$1.6936 \cdot 10^{-3}$	$1.6938 \cdot 10^{-3}$	0.0128%
Terrestrial ecotoxicity	kg 1,4-DB eq	$1.0923 \cdot 10^{-3}$	$1.0924 \cdot 10^{-3}$	0.0071%

Mean Error 0.0015%

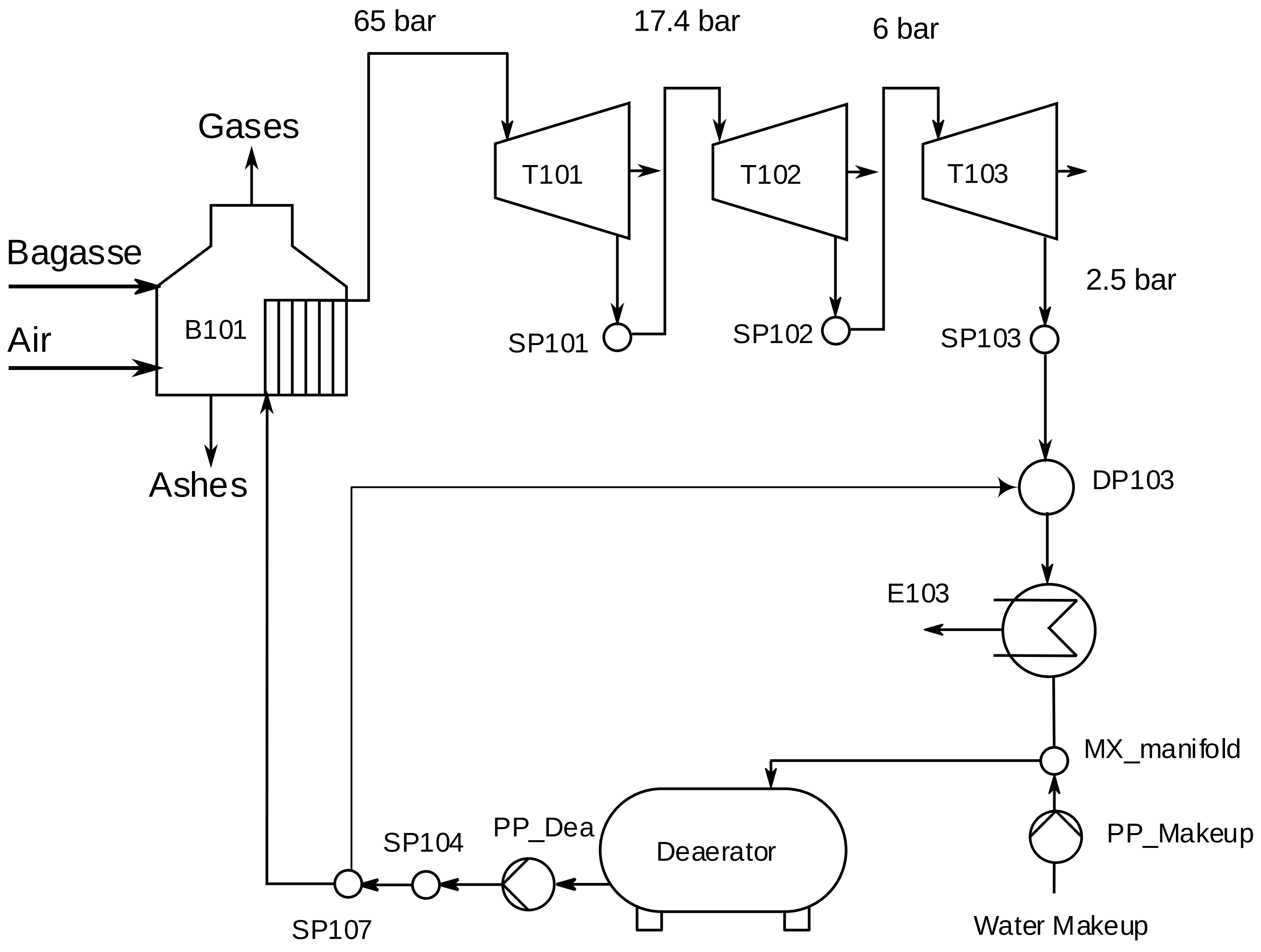
Bioeletricity and Steam Co-generation

Premisses

- Availability of 129 kt/h of sugarcane bagasse and straw for cogeneration
- Demand of vapor: 113.5 MWh (DIAS et al. 2013)
- Boiler efficiency: 87,2% (DIAS et al. 2013)
- Outlet Boiler temperature of Gases: 160ºC (Dias et al. 2013)
- Pressure and temperature of the boiler outlet steam: 65bar e 485ºC (DIAS et al. 2013)
- Air excess: 30% (DIAS, 2011)
- Steam Loss: 4%
- Pump Efficiency: 70%
- Turbine Efficiency: 0.85%
- Mechanical Efficiency:0.98%
- C price: 43US$/t
- Electricity Price: 59.50 US$/MWh
- Water Price: 0.005235 US$/kg
- Vapor Price= $\left(\frac{Electricity\ Revenue - Water\ Cost + Carbon\ Credit\ (or\ Cost)}{Vapor\ consumption\ (MWh)}\right)$
- Efficiency = $\left(\frac{Net\ Electricity + vapor}{Heat\ available\ to\ the\ boiler}\right)$

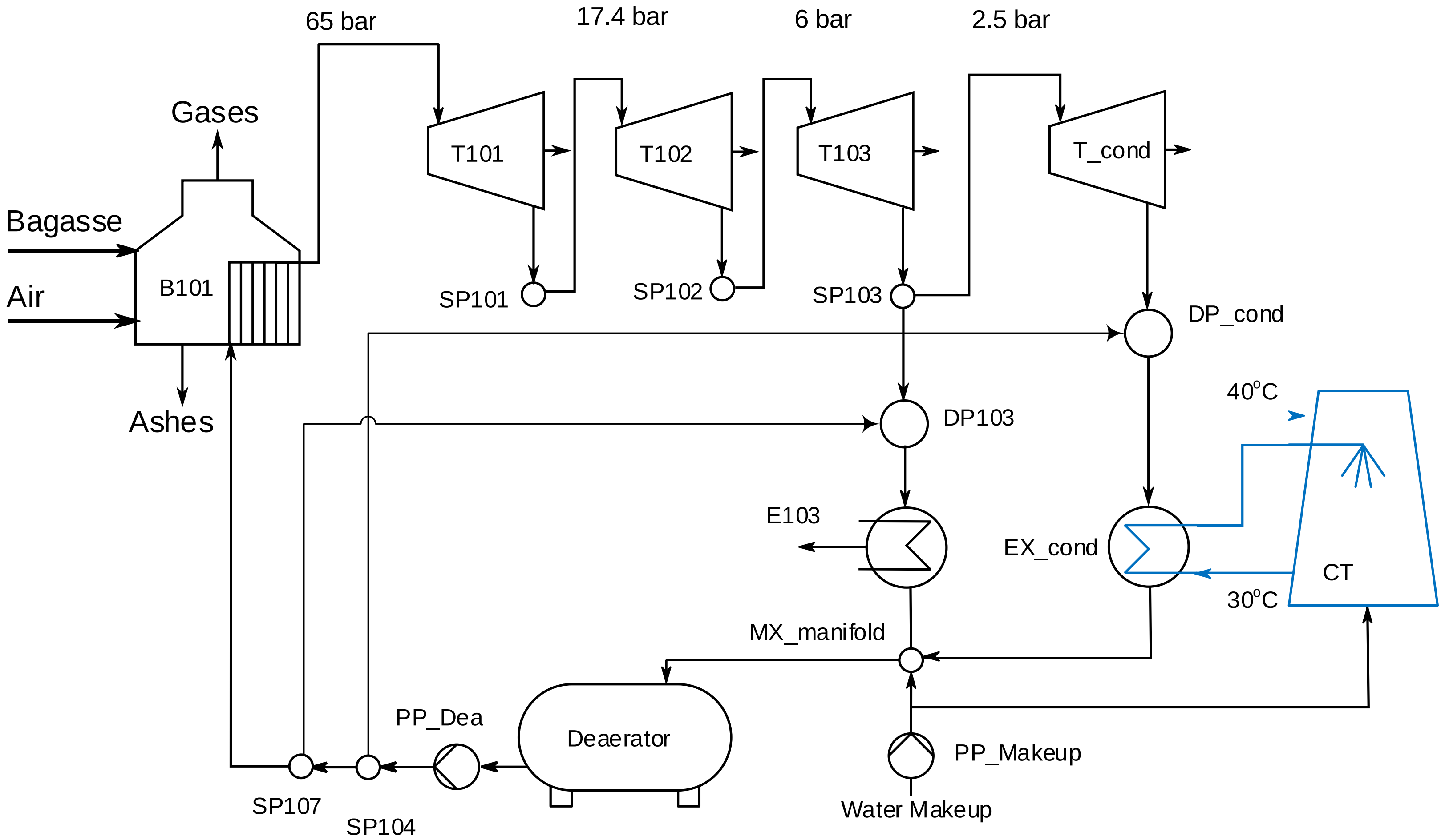
Bioelectricity and Steam Co-generation

Scenario 1



Bioelectricity and Steam Co-generation

Scenario2



Bioelectricity and Steam Co-generation

Emission on Boiler

Emissions[1]	Elementary Flow [2]	Elementary Flow Path1 [2]	Value[1]	Unit
VOC	NMVOC	Emission to air	0.00761463	kg/t
CO	Carbon monoxide	Emission to air	0.120739025	kg/t
NO	Nitrogen oxides	Emission to air	0.795076714	kg/t
PM2.5	Particulates, < 2.5 um	Emission to air	0.015689025	kg/t
PM10	Particulates, < 10um	Emission to air	0.017764133	kg/t
SO	Sulfur oxides	Emission to air	0.729576105	kg/t
BC	Black Carbon	Emission to air	0.002165085	kg/t
OC	Organic Carbon	Emission to air	0.005114622	kg/t
CH_4	Methane	Emission to air	0.122146171	kg/t
NO_2	Dinitrogen monoxide	Emission to air	0.075615476	kg/t
CO_2	Carbon dioxide, biogenic	Emission to air	from simulation	-

Source: [1] Greet (2022) [2] OpenLCA (2022)

Bioelectricity and Steam Co-generation LCA

1. The inventory for both scenarios for 113.5 MWh of 2.5 bar steam was estimated;
2. The LCA was calculated for each scenario considering the inventory above;
3. Then it was estimated the contribution of the inputs and the emissions to the results;
4. Still, it was assessed the impact on the variation of the consumed vapor on Carbon Credit, GWP, efficiency and vapor cost.

Cogeneration Study Case
Inventory Results

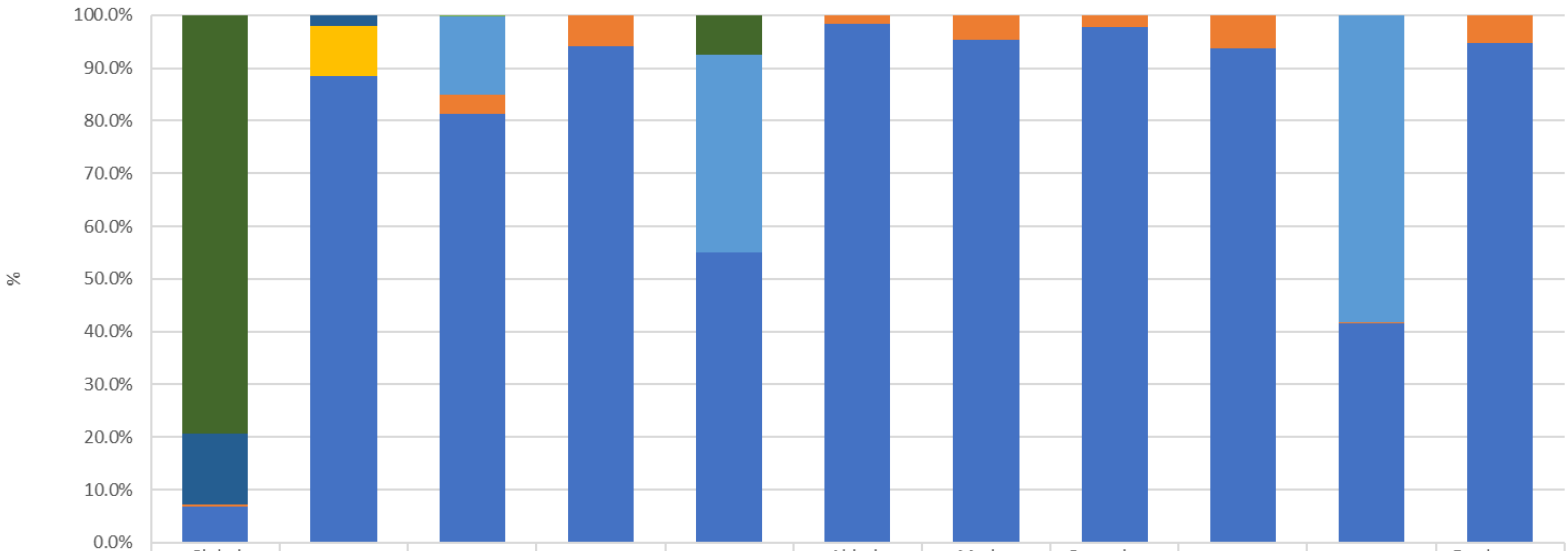
Inventory	Unit	Scenario 1	Scenario 2	Δ%
Inputs				
Bagasse/Straw	t/h	38.04	129.06	339%
Water	t/h	7.46	479.56	6433%
Emissions				
VOC	kg/h	0.32	1.08	339%
CO	kg/h	5.06	17.18	339%
NO	kg/h	33.34	113.11	339%
Particulate M., < 2,5 um	kg/h	0.66	2.23	339%
Particulate M., < 10um	kg/h	0.74	2.53	339%
SO	kg/h	30.59	103.79	339%
BC	kg/h	0.09	0.31	339%
OC	kg/h	0.21	0.73	339%
CH_4	kg/h	5.12	17.38	339%
N_2O	kg/h	3.17	10.76	339%
CO_2, biogenic	t/h	61.56	208.87	339%
Products				
Vapor	MWh	113.50	113.50	100%
Bioeletricity, net	MWh	34.02	154.38	454%

Cogeneration Study Case
LCA Results

Impact Category	Unit	Scenario 1	Scenario 2	Δ%
Global Warming (GWP100a)	kg CO_2 eq/MJ	$1.995 \cdot 10^{-3}$	$4.033 \cdot 10^{-3}$	202%
Photochemical oxidation	kg C_2H_4 eq/MJ	$2.761 \cdot 10^{-6}$	$5.285 \cdot 10^{-6}$	191%
Human toxicity	kg 1,4-DB eq/MJ	$5.087 \cdot 10^{-4}$	$1.571 \cdot 10^{-3}$	309%
Abiotic depletion	kg Sb eq/MJ	$7.270 \cdot 10^{-9}$	$2.776 \cdot 10^{-8}$	382%
Eutrophication	kg PO_4-eq/MJ	$2.172 \cdot 10^{-5}$	$4.120 \cdot 10^{-5}$	190%
Abiotic depletion (fossil fuels)	MJ/MJ	$5.979 \cdot 10^{-3}$	$1.448 \cdot 10^{-2}$	242%
Marine aquatic ecotoxicity	kg 1,4-DB eq/MJ	$4.470 \cdot 10^{-1}$	1.533E+00	343%
Ozone layer depletion (ODP)	kg CFC-11 – eq/MJ	$3.558 \cdot 10^{-11}$	9.244E-11	260%
Terrestrial ecotoxicity	kg 1,4-DB eq/MJ	$1.955 \cdot 10^{-6}$	7.737E-06	396%
Acidification	kg SO_2-eq/MJ	$5.381 \cdot 10^{-5}$	1.026E-04	191%
Fresh water aquatic ecotox.	kg 1,4-DB eq/MJ	$2.411 \cdot 10^{-4}$	8.787E-04	364%

Cogeneration Study Case

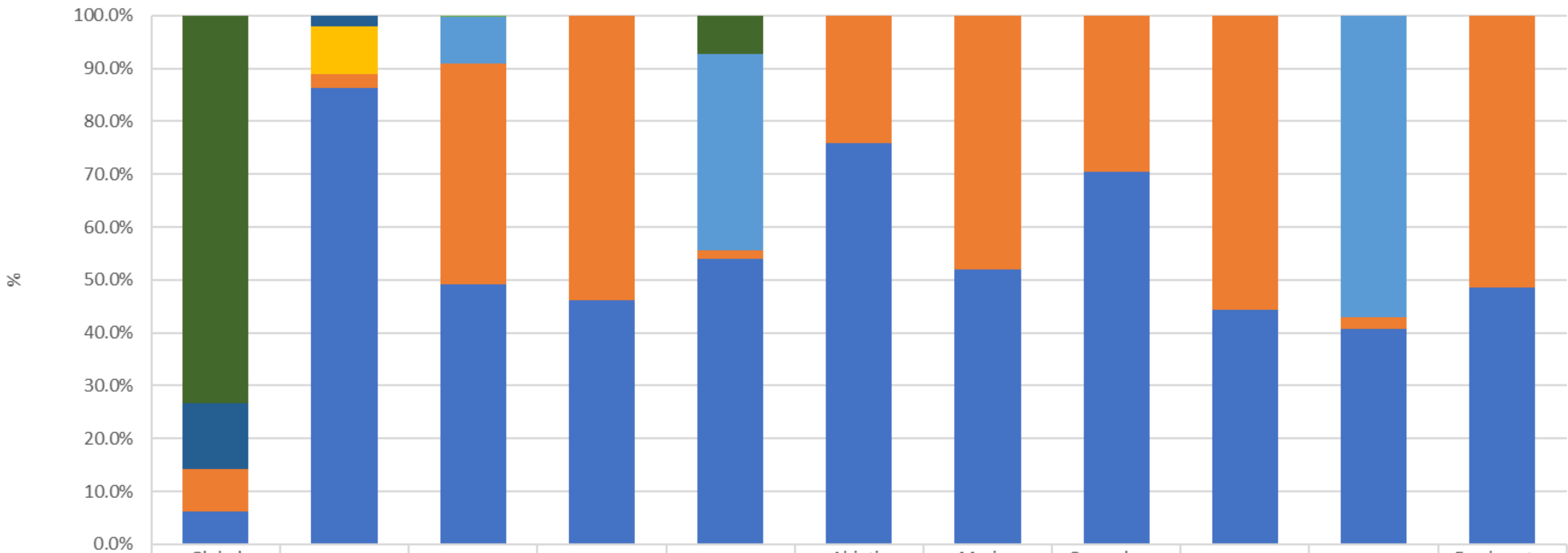
Contribution of Inputs and Emissions on Result – Scenario 1



	Global warming (GWP100a)	Photochemical oxidation	Human toxicity	Abiotic depletion	Eutrophication	Abiotic depletion (fossil fuels)	Marine aquatic ecotoxicity	Ozone layer depletion (ODP)	Terrestrial ecotoxicity	Acidification	Fresh water aquatic ecotox.
CO2, Biogenic	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
N2O	79.3%	0.0%	0.0%	0.0%	7.4%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
CH4	13.5%	2.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
OC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
BC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
SO	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
PM10	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
PM25	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
NO	0.0%	0.0%	14.8%	0.0%	37.6%	0.0%	0.0%	0.0%	0.0%	58.3%	0.0%
CO	0.0%	9.3%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
VOC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Water	0.5%	0.1%	3.6%	5.8%	0.1%	1.6%	4.7%	2.2%	6.2%	0.1%	5.3%
Bagasse	6.7%	88.4%	81.4%	94.2%	54.9%	98.4%	95.3%	97.8%	93.8%	41.6%	94.7%

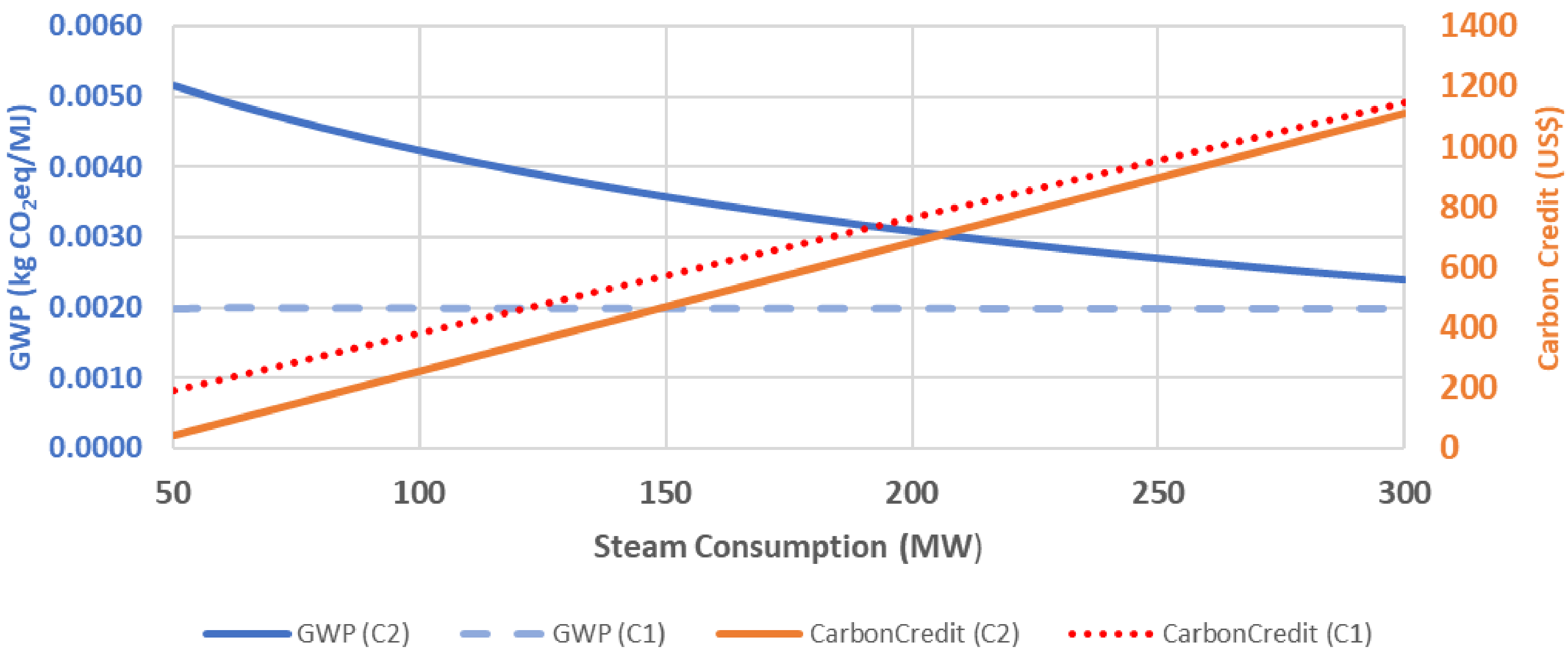
Cogeneration Study Case

Contribution of Inputs and Emissions on Result – Scenario 2

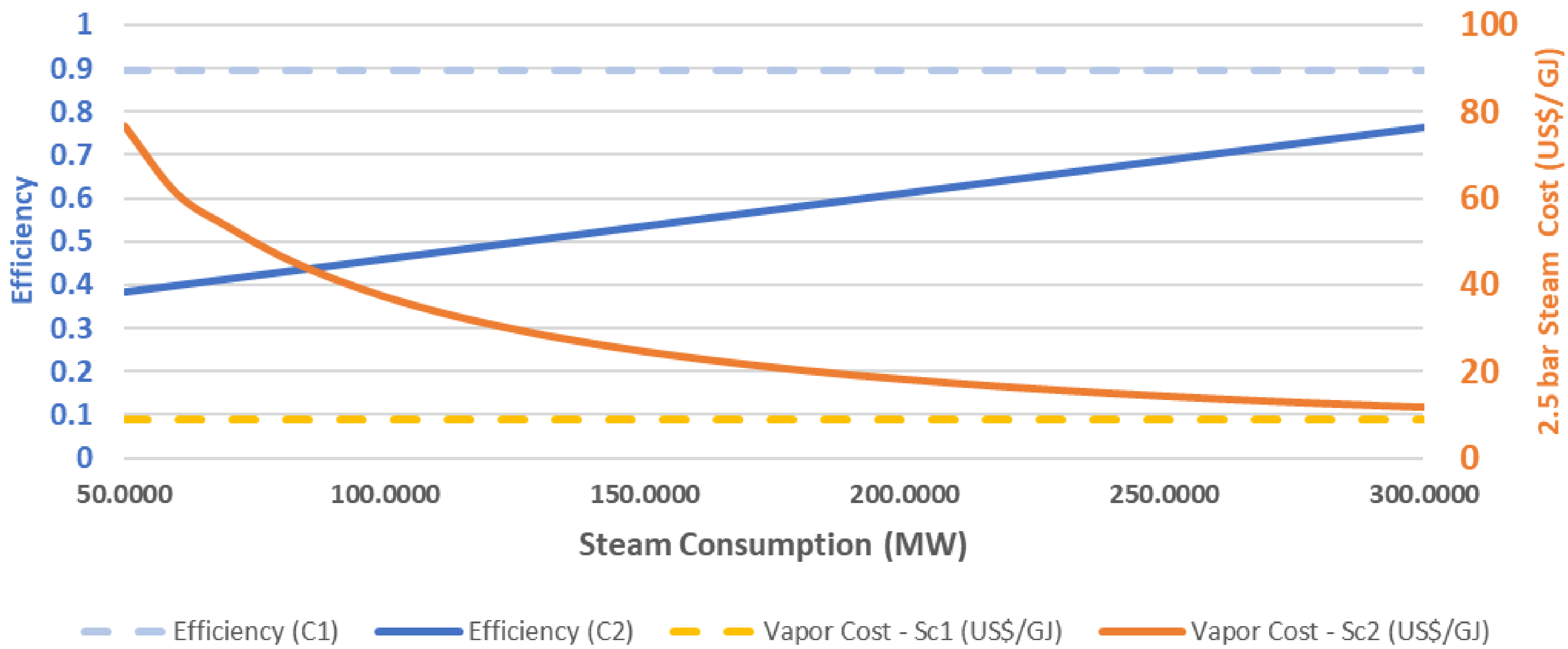


	Global warming (GWP100a)	Photochemical oxidation	Human toxicity	Abiotic depletion	Eutrophication	Abiotic depletion (fossil fuels)	Marine aquatic ecotoxicity	Ozone layer depletion (ODP)	Terrestrial ecotoxicity	Acidification	Fresh water aquatic ecotox.
CO2, Biogenic	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
N2O	73.3%	0.0%	0.0%	0.0%	7.3%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
CH4	12.5%	2.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
OC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
BC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
SO	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
PM10	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
PM25	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
NO	0.0%	0.0%	9.0%	0.0%	37.0%	0.0%	0.0%	0.0%	0.0%	57.1%	0.0%
CO	0.0%	9.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
VOC	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Water	8.0%	2.5%	41.7%	53.9%	1.6%	24.1%	48.1%	29.6%	55.7%	2.2%	51.5%
Bagasse	6.2%	86.4%	49.2%	46.1%	54.1%	75.9%	51.9%	70.4%	44.3%	40.7%	48.5%

Cogeneration Study Case
Case Study Results
Effect on GWP and Carbon Credit , varying Steam Consumption



Cogeneration Study Case
Case Study Results
Effect on Efficiency and Vapor Cost, varying Steam Consumption



Conclusions

- A platform for integration of OpenLCA and EMSO was implemented.
- Due to its framework, it presented flexibility, computational speed compatible with the use of simulators (0.296 s), Accuracy of the calculations (0.0015%) compared to OpenLCA.
- The integration of OpenLCA with EMSO allows the user to implement more complexes LCAs.
- As the communication is direct with the OpenLCA database, it minimize human errors on calculations, and guarantee that the database presents consistent data as it elaborated by OpenLCA;
- In the Cogeneration Case, the EMSO_OLCA showed robustness on calculations and was fully integrated with others EMSO entities as Case Study.
- In the Cogeneration Case, the EMSO_OLCA allowed to show which process configuration presented lower environmental impact and lower cost. In this case the reduction of environmental impact goes to the same direction as the economic ones.
- The Cogeneration study also showed that if the steam generated is not directly used in the process, it is not worthy a condensation turbine even if it produces more electricity.