Life Cycle Assessment integrated to process simulator EMSO

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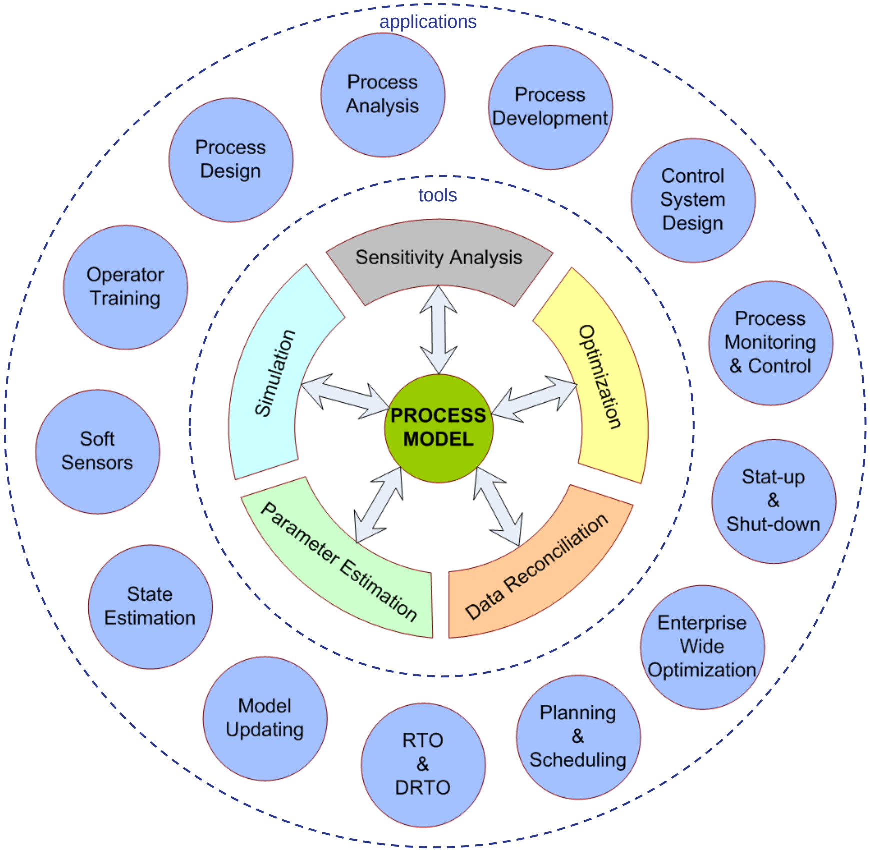
Outline

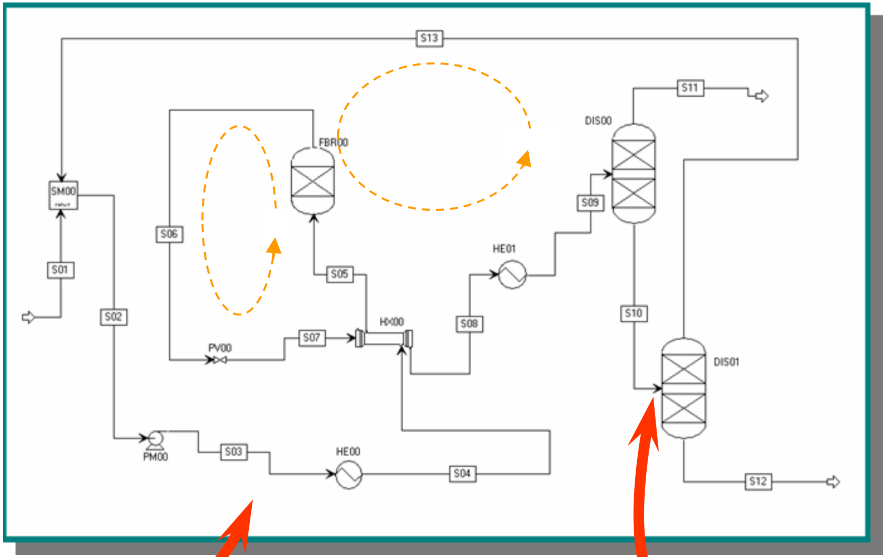
1. **Introduction**
2. **Introducing EMSO**
3. **Life Cycle Assessment**
4. **EMSO_OLCA**
5. **Applications**

Applications of Process Modeling



Sequential Modular Simulators

- **Sequential Modular Simulators**

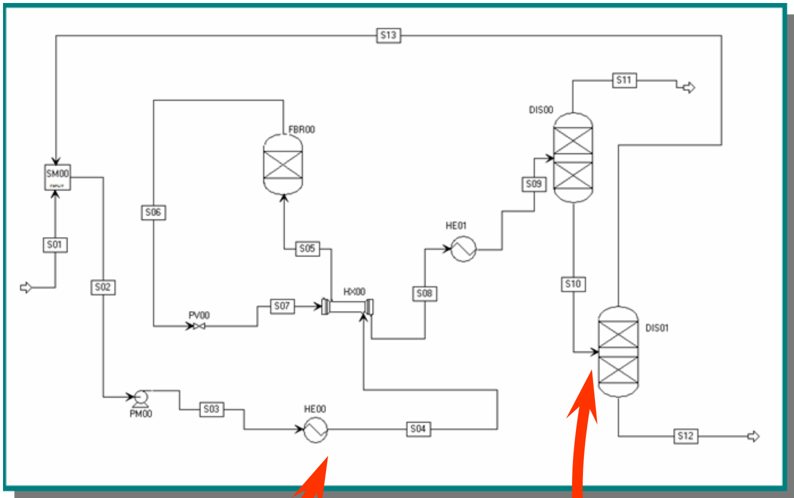


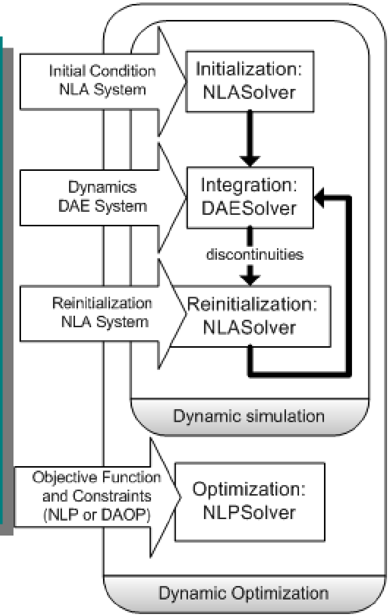
ex: AspenPlus, Hysys, PRO/II, Chemcad, Petrox

Black Box Modeling

The code is specific for every equipment

Equation-Oriented Simulators





Open-source
Modeling

Equipments contain only chemistry and physics of the model

All equipments or modules are simultaneously evaluated (Block decomposition can be used to explore sequential solution)

ex: EMSO, Ascend, Jacobian, gPROMS, AspenDynamics, EcosimPro

Object-oriented modeling

Examples of general-purpose object-oriented modeling languages:

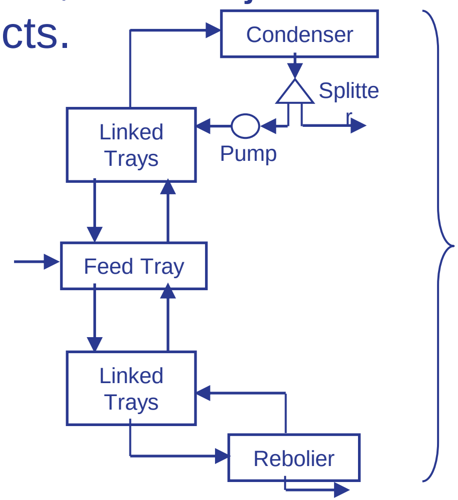
- ABACUSS II (Barton, 1999)
- ASCEND (Piela, 1989)
- Dymola (Elmqvist, 1978)
- EcosimPro (EA Int. & ESA, 1999)
- EMSO (Soares and Secchi, 2003)
- gPROMS/Speedup (Barton and Pantelides, 1994)
- Modelica (Modelica Association, 1996)
- ModKit (Bogusch et al., 2001)
- MPROSIM (Rao et al., 2004)
- Omola (Andersson, 1994)
- ProMoT (Tränkle et al., 1997)

Object-oriented modeling

OOM main concepts

Inheritance: is the process whereby one object acquires (gets, receives) characteristics from one or more other objects.

Aggregation: is the process of creating a new object from two or more other objects, or an object that is composed of two or more other objects.



Column model = Condenser + Splitter + Pump + Linked Trays + Feed Tray + Reboiler

EO CAPE Tools

- Key advantages of EO:
  - Models can be inspected, refined, or reused
  - Easier to diagnose ill-posed problems
  - Same model as the source for several tasks: simulation, optimization, design, parameter estimation, data reconciliation, etc. → integrated environment

- Some disadvantages:
  - More difficult to establish good initial guesses
  - More demand on computer resources

ALSOC PROJECT - EMSO - Trac - Mozilla Firefox

Arquivo Editar Exibir Histórico Favoritos Ferramentas Ajuda

http://www.enq.ufrgs.br/trac/alsoc

New Group | New Group (1)

ALSOC PROJECT - EMSO - Trac

Welcome to the ALSOC Project homepage

ALSOC is the acronym used to identify the project of a free environment for simulation, optimization, and process control.
ALSOC é a sigla utilizada para identificar o projeto de um **A**mbiente **L**ivre para **S**imulação, **O**timização e **C**ontrole de Processos.

The ALSOC Project is an effort to bring together university-industry through the standardization and distribution without cost of specifications and software tools among universities and partner companies.
O Projeto ALSOC é um esforço de aproximação universidade-indústria através da padronização e distribuição sem custo de especificações e ferramentas de software entre universidades e empresas consorciadas.

Look here the list of institutions that **participate** and **sponsor** the project.
Veja aqui a lista de instituições que **participam** e **patrocinam** o projeto.

Project Goals

The main goals of the ALSOC Project are:
As principais finalidades do Projeto ALSOC são:

- to develop, maintain, and distribute specifications of a modeling language and a library of models for the synthesis, simulation, optimization and control of general processes (check the ALSOC OPEN LICENSE);
  desenvolver, manter e distribuir especificações de uma linguagem de modelagem e uma biblioteca de modelos abertas para síntese, simulação, otimização e controle de processos em geral (veja a licença aberta ALSOC);
- to develop and maintain state-of-the-art software and to distribute it at no cost to the universities and partner companies (check the ALSOC LICENSE);
  desenvolver e manter software no estado-da-arte distribuído sem custo entre os consorciados e entidades educacionais (veja a licença ALSOC);
- to certify third party solution and models as conforming to the developed standards.
  certificar a conformidade de soluções externas com os padrões desenvolvidos e adicionar ao Projeto contribuições externas.

EMSO Process Simulator

EMSO is the acronym for Environment for Modeling Simuation and Optimization.
EMSO é a sigla para *Environment for Modeling Simuation and Optimization*.

EMSO is the simulation software of the ALSOC project. Its development was started at 2001 by Rafael de Pelegrini Soares, today the EMSO process simulator is developed and maintained by ALSOC.
O EMSO é o *software* de simulação do projeto ALSOC. Sua construção foi iniciada em 2001 por Rafael de Pelegrini Soares, hoje o simulador EMSO é desenvolvido e mantido pelo projeto ALSOC.

Learn more about EMSO, check the ChangeLog, or download it here!
Saiba mais sobre o EMSO, veja o ChangeLog ou faça o seu download aqui!

News!

- **mar 07 2008**: EMSO **version 0.9.55** released! Download it here
- **dez 25 2007**: EMSO **version 0.9.54** released! Download it here
- **aug 31 2007**: EMSO **version 0.9.53** released! Download it here
- **aug 27 2007**: Curso do simulador EMSO. Clique AQUI para fazer o download do material do curso.
- **jun 15 2007**: A nice Quick Reference is now available.
- **feb 14 2007**: Displaying a formula Click here.
- **dec 18 2006**: **ALSOC meeting**: sponsors and developers discussing about the future of the project and recent advances. Read more...
- **nov 1 2006**: **Get involved!**: Contribute your models to the EMSO Model Library. Check the Contribution Page!

DEQUI - Departamento de ENGENHARIA QUÍMICA

GIMSCOP

Concluído

ALSOC Project

Industry-University Partnership (2004-2009):

UFRGS

COPPE/UFRJ

USP

MACKENZIE

FINEP-CNPq

PETROBRAS

BRASKEM

COPESUL

INNOVA

IPIRANGA

P. TRIUNFO

REFAP

ALSOC Project

Collaborators Universities

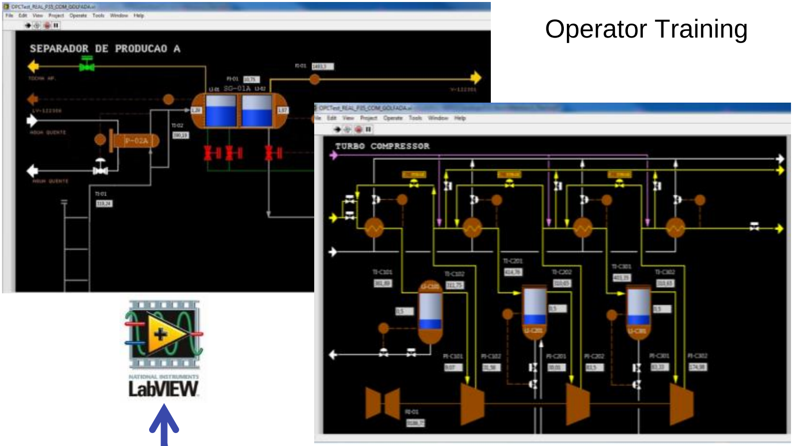
UFRG
S

UFBa

UFU

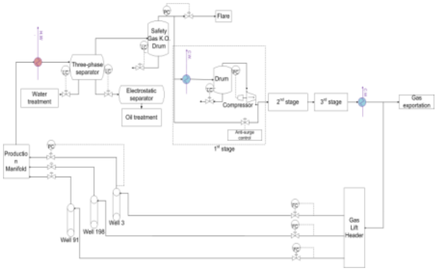
EMSO Applications:

Operator Training



FPSO

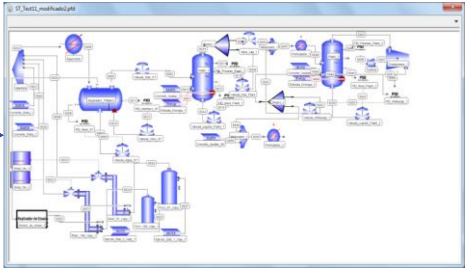
PFD



OPC Server

EMSO OPC

Simulation - EMSO



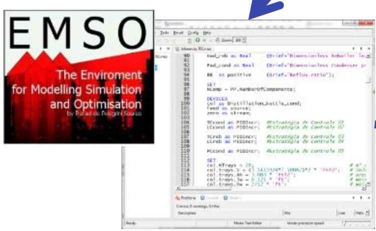
Soft Sensor:

Especification of GLP

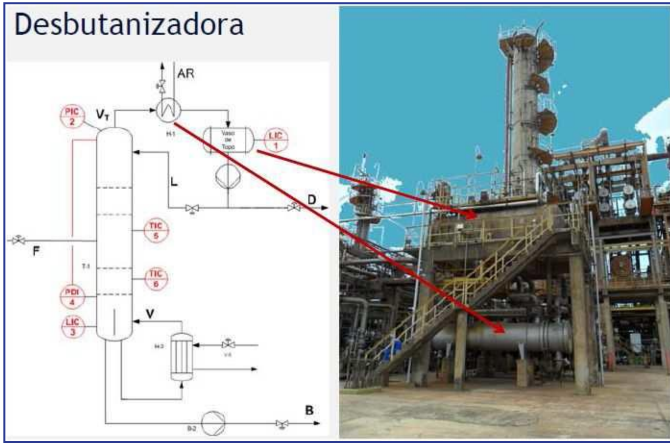
GLP: C2 (11%)
C3
C4
C5 (1,5%)

Plant

Reflux
Temperature of the Bottom
Pressure



FlowSheet EMSO



Inference (min a min) x Measurements (20 min)

Composition of C5
In top of the column

Model Building

✓ **A mathematical model has:**

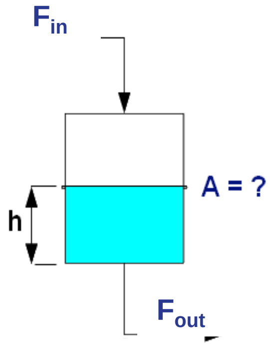
- A set of model parameters (reaction order, valve constant, etc.)
- A set of variables (temperatures, pressures, flow rates, etc.)
- A set of equations (algebraic and differential) relating the variables

✓ **Problems in model building:**

- Number of equations and variables do not match (DoF $\neq$ 0)
- Equations of the model are inconsistent (linear dependence, UOM, etc.)
- The number of initial conditions and DDoF do not match

The Simplest Example

Abstract model



mass balance: $F_{in} - F_{out} = \frac{dV}{dt}$

valve equation: $F_{out} = k\sqrt{h}$

liquid volume: $V = A\,h$

EMSO:

```
using "types";
Flowsheet basic_flowsheet
PARAMETERS
    k as Real (Brief="Valve constant", Unit='m^2.5/h', Default = 12);
    D as length (Brief="Tank hydraulic diameter", Default = 4);
VARIABLES
     Fin as flow_vol (Brief="Feed flow rate");
     Fout as flow_vol (Brief ="Output flow rate");
     A as area (Brief="Cross section area");
     V as volume (Brief="Liquid volume");
     h as length (Brief="Tank level");
EQUATIONS
    "Mass balance"  Fin - Fout = diff(V);  # (1)
    "Valve equation" Fout = k * sqrt(h);  # (2)
    "Liquid volume"  V = A * h;            # (3)
end
```

Modeling
Consistency Analysis

- Model consistency analysis for unit of measurements (UOM)
- Degree of freedom analysis
- Dynamic degree of freedom analysis

<u>variable</u>	<u>UOM</u>
F_{in}, F_{out}	$m^3\ h^{-1}$
V	m^3
A	m^2
h	m
k	$m^{2.5}\ h^{-1}$
t	h

<u>equations</u>

(1): $[m^3\ h^{-1}] - [m^3\ h^{-1}] = [m^3] / [h]$

(2): $[m^3\ h^{-1}] = [m^{2.5}\ h^{-1}]\ ([h])^{0.5}$

(3): $[m^3] = [m^2]\ [m]$

Modeling
Consistency Analysis

variables: F_{in}, F_{out}, V, A, h, k, t ➔ 7

constants: k, A ➔ 2

specifications: t ➔ 1

driving forces: F_{in} ➔ 1

unknown variables: V, h, A, F_{out} ➔ 4

equations: 3

Degree of Freedom = variables – constants – specification – driving forces – equations = unknown variables – equations = 7 – 2 – 1 – 1 – 3 = 0

Dynamic Degree of freedom (index < 2) = differential equations = 1

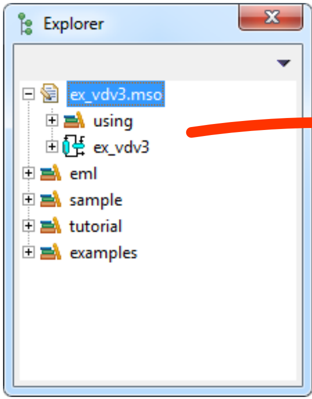
Needs 1 initial condition: h(0) ➔ 1

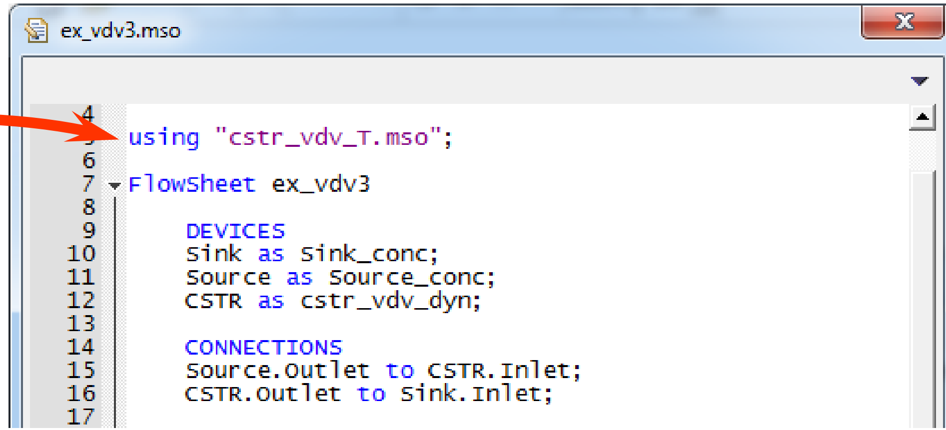
```
using "types";
constante as Real (Unit = 'm^2.5/h’);

Flowsheet meuprimeirotanque
PARAMETERS
K as constante;
A as area;

VARIABLES
V as volume;
h as length;
Fe as flow_vol;
Fs as flow_vol;

EQUATIONS
diff(V) = Fe - Fs;
V = A * h;
Fs = K * sqrt(h);
SET
K = 5 * 'm^2.5/h’;
A = 1 * 'm^2’;
SPECIFY
Fe = 2 * (1 + sin(40*time*'rad/h')) * 'm^3/h’;
#Fe = 2 * 'm^3/h’;

INITIAL          h = 0.5 * 'm';
```

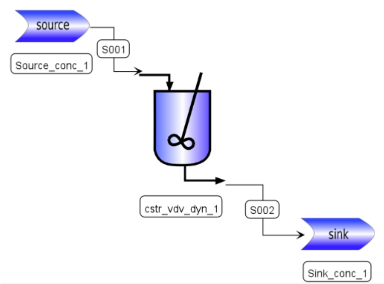
My first EMSO Simulation Hello World!

```
OPTIONS
TimeStart = 0;
TimeStep = 0.01;
TimeEnd = 1.5;
TimeUnit = 'h';
```

Modeling Structure in EMSO







1. Definições dos Equipamentos
2. Conexões

Modeling Structure in EMSO

using reference to files.

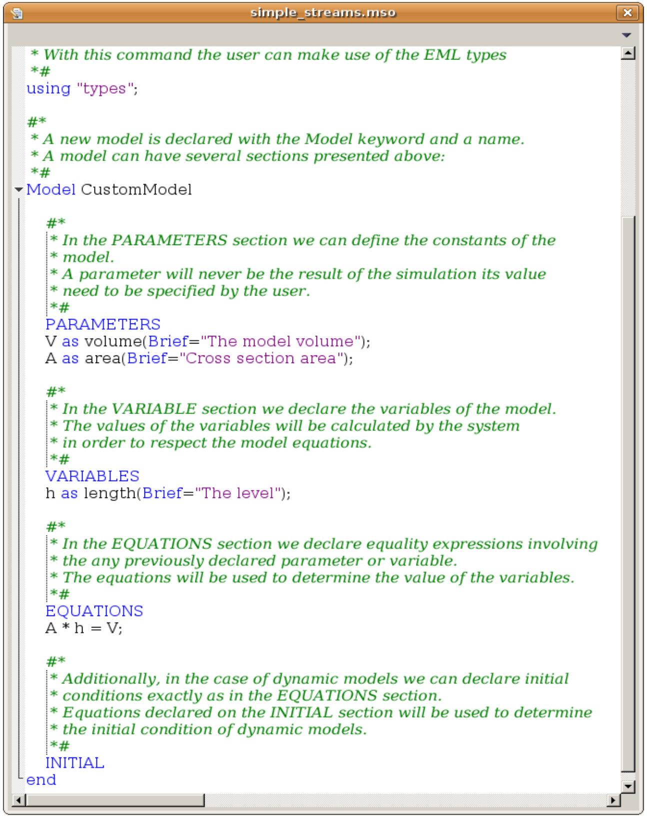
Model a new model is set with this word

the new model should have:

PARAMETERS parameters section of the model.

VARIABLES variables section of the model.

EQUATIONS equations section of the model



```
 * With this command the user can make use of the EML types
 *#
using "types";

#*
 * A new model is declared with the Model keyword and a name.
 * A model can have several sections presented above:
 *#
Model CustomModel

    #*
    * In the PARAMETERS section we can define the constants of the
    * model.
    * A parameter will never be the result of the simulation its value
    * need to be specified by the user.
    *#
    PARAMETERS
    V as volume(Brief="The model volume");
    A as area(Brief="Cross section area");

    #*
    * In the VARIABLE section we declare the variables of the model.
    * The values of the variables will be calculated by the system
    * in order to respect the model equations.
    *#
    VARIABLES
    h as length(Brief="The level");

    #*
    * In the EQUATIONS section we declare equality expressions involving
    * the any previously declared parameter or variable.
    * The equations will be used to determine the value of the variables.
    *#
    EQUATIONS
    A * h = V;

    #*
    * Additionally, in the case of dynamic models we can declare initial
    * conditions exactly as in the EQUATIONS section.
    * Equations declared on the INITIAL section will be used to determine
    * the initial condition of dynamic models.
    *#
    INITIAL
end
```

Componentes Básicos do Modelo

Submodels and predefined EMSO models

Information for documentation

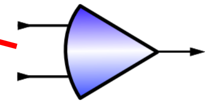
Basic Section

Of the model

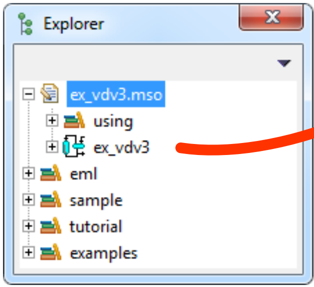
Inlet and Outlet Conections

mixer.mso

```
using "streams";

Model mixer
	ATTRIBUTES
	Pallete 	= true;
	Icon 		= "icon/mixer";
	Brief 		= "Model of a mixer";
	Info 		=
"== Assumptions ==
* static
* adiabatic

== Specify ==
* the inlet streams";

	PARAMETERS
outer NComp as Integer (Brief = "Number of chemical components", Lower = 1);
	NInlet as Integer (Brief = "Number of Inlet Streams", Lower = 1, Default = 2);

	VARIABLES
in	Inlet(NInlet) as stream (Brief = "Inlet streams", PosX=0, PosY=0.5, Symbol="_{in}");
out	Outlet 		as streamPH (Brief = "Outlet stream", PosX=1, PosY=0.5, Symbol="_{out}");

	EQUATIONS

	"Flow"
	Outlet.F = sum(Inlet.F);

	for i in [1:NComp]

		"Composition"
		Outlet.F*Outlet.z(i) = sum(Inlet.F*Inlet.z(i));
	end

	"Energy Balance"
	Outlet.F*Outlet.h = sum(Inlet.F*Inlet.h);

	"Pressure"
	Outlet.P = min(Inlet.P);
end
```



Modeling Structure in EMSO




```
#*-------------------------------------------------
* FlowSheet generated automaticaly by EMSO-GUI
*------------------------------------------------*#

using "cstr_vdv_T.mso";

FlowSheet ex_vdv3

	DEVICES
	Sink as Sink_conc;
	Source as Source_conc;
	CSTR as cstr_vdv_dyn;

	CONNECTIONS
	Source.Outlet to CSTR.Inlet;
	CSTR.Outlet to Sink.Inlet;

	SET
	CSTR.cv = 1 * 'm^(5/2)/h' ;
	CSTR.k1 = 1.287E+012 * '1/h' ;
	CSTR.k2 = 1.287E+012 * '1/h' ;
	CSTR.k3 = 9.043E+009 * 'l/mol/h' ;
	CSTR.E1 = 9758.3 * 'K' ;
	CSTR.E2 = 9758.3 * 'K' ;
	CSTR.E3 = 8560 * 'K' ;
	CSTR.A = 1 * 'm^2' ;

	SPECIFY
	Source.Outlet.Ca = 5.5 * 'kmol/m^3' ;
	Source.Outlet.Cb = 0 * 'kmol/m^3' ;
	Source.Outlet.Cc = 0 * 'kmol/m^3' ;
	Source.Outlet.Cd = 0 * 'kmol/m^3' ;
	Source.Outlet.T = 387 * 'K' ;
	Source.Outlet.P = 1 * 'atm' ;
	Source.Outlet.Fvol = 1 * 'm^3/h' ;
	CSTR.x = 1 ;

	INITIAL
	CSTR.Ca = 5 * 'kmol/m^3' ;
	CSTR.Cb = 0 * 'kmol/m^3' ;
	CSTR.Cc = 0 * 'kmol/m^3' ;
	CSTR.Cd = 0 * 'kmol/m^3' ;
	CSTR.h = 1 * 'm' ;
```

EQUIPAMENTS parameters

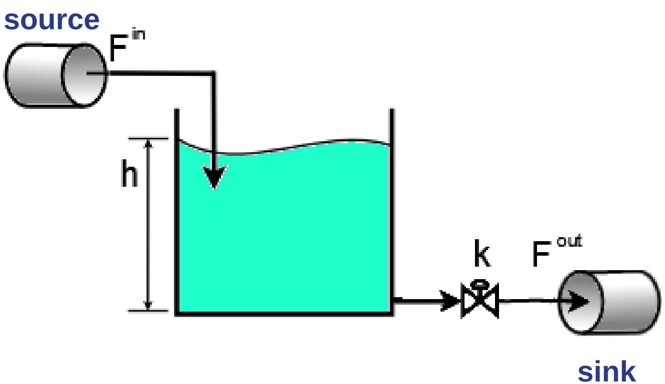
Degree of freedom

Dynamic Degree of freedom

```
OPTIONS
Dynamic = true;
TimeStep = 0.01;
TimeEnd = .5;
TimeUnit = 'h';
Integration = "original";
NLASolver(
	File = "sundials",
	RelativeAccuracy = 1e-6,
	AbsoluteAccuracy = 1e-6,
	MaxIterations = 100
);
DAESolver(
	File = "dasslc",
	RelativeAccuracy = 1e-6,
	AbsoluteAccuracy = 1e-6,
	EventAccuracy = 1e-2
);
```

Simulation Options

Simple Example



Level Tank

<u>Streams</u>

Inlet	stream feeding the tank
Outlet	stream leaving the tank

<u>Parameters</u>

K	Valve constant

<u>Variables</u>

A	Tank cross section area
V	Tank volume
h	Tank level

<u>Devices:</u> source, tank, sink

Creating Models

```
using "types";

# Source model
Model Feed
  VARIABLES
  out F as flow_vol;
end

# Sink model
Model Sink
  VARIABLES
  in F as flow_vol;
end
```

Creating Models

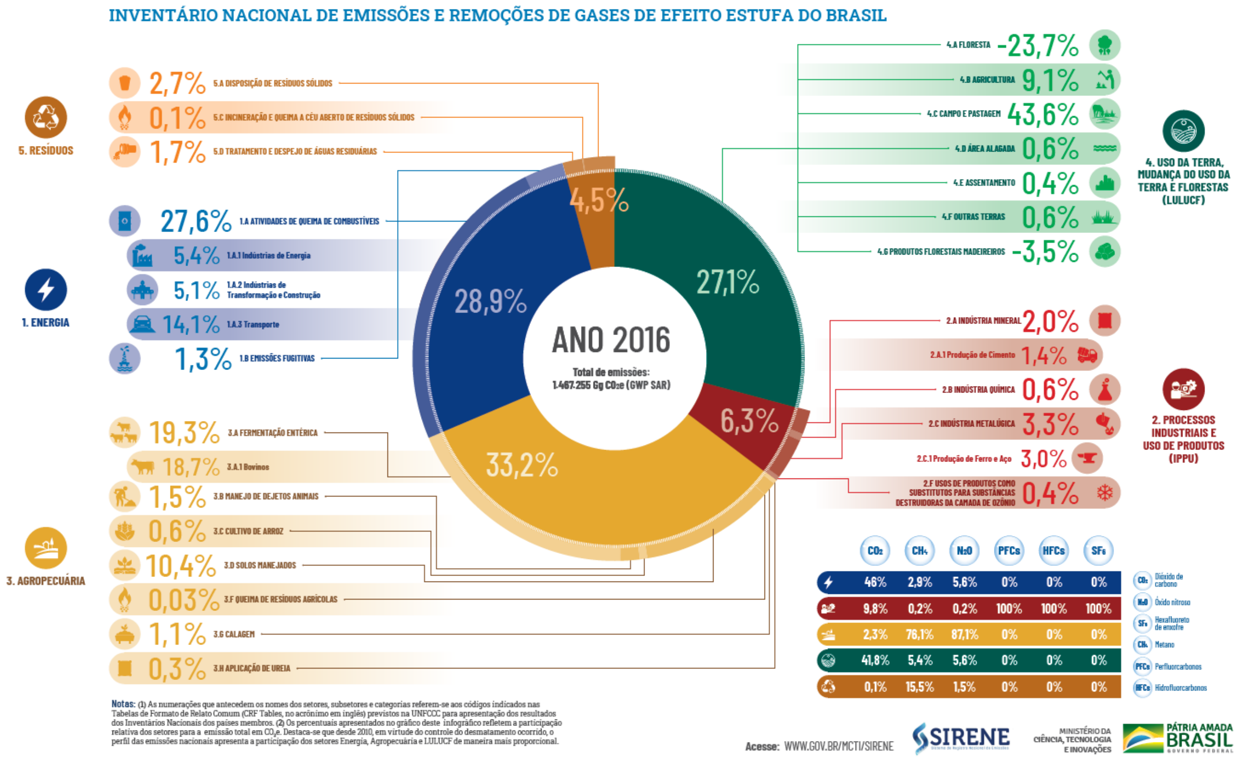
```
Model Tank_Basic
PARAMETERS
K as Real;

VARIABLES
in  Fin as flow_vol;
out Fout as flow_vol;
V as volume;
h as length;
A as area;

EQUATIONS
Fin - Fout = diff(V);
Fout = K * sqrt(h);
V = A * h;
end
```

Creating Models

```
FlowSheet meusegundotanque
DEVICES
Tank1 as Tank_Basic;
Input as Feed;
Output as Sink;

CONNECTIONS
Input to tanque1;
Tank1 to Output;

SET
Tank1.K = 5 * 'm^2.5/h’;
Tank1.A = 1 * 'm^2’;

SPECIFY
Input.F = 2 * (1 + sin(40*time*'rad/h')) * 'm^3/h';
INITIAL
Tank1.h = 0.5 * 'm’;
OPTIONS
TimeStart = 0;
TimeStep = 0.01;
TimeEnd = 1.5;
TimeUnit = 'h’;
end
```

Life Cycle Assessment

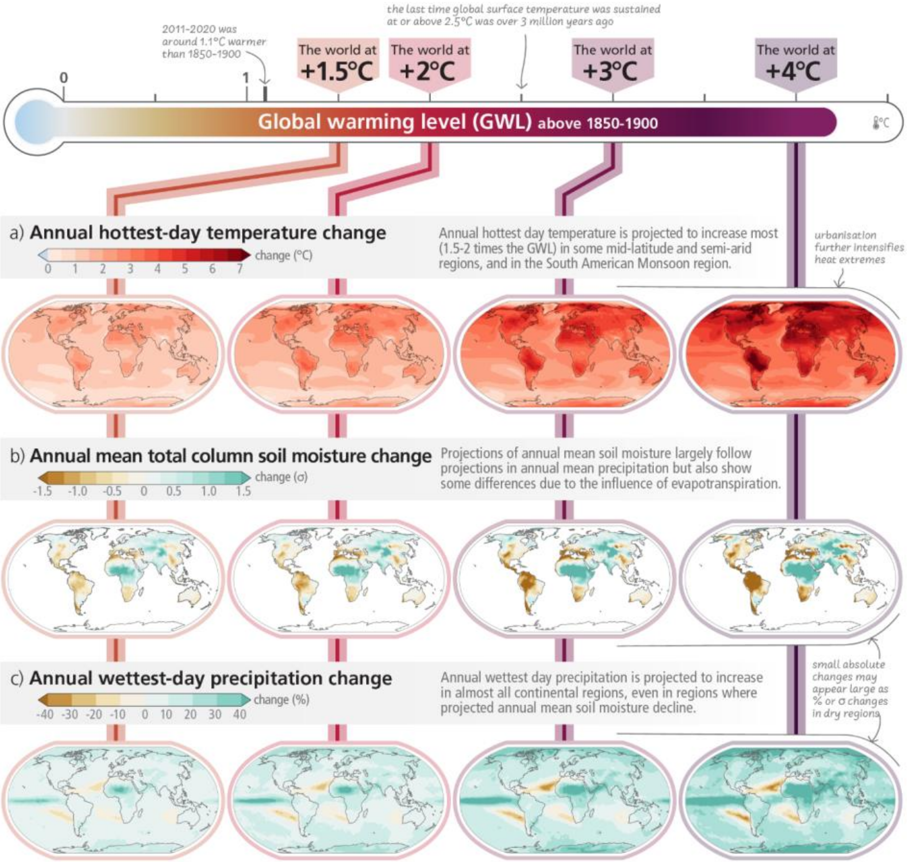
Life Cycle Assessment



	CO_2	CH_4	N_2O	PFCs	HFCs	SF_6
1. Energia	46%	2,9%	5,6%	0%	0%	0%
2. IPPU	9,8%	0,2%	0,2%	100%	100%	100%
3. Agropecuária	2,3%	76,1%	87,1%	0%	0%	0%
4. LULUCF	41,8%	5,4%	5,6%	0%	0%	0%
5. Resíduos	0,1%	15,5%	1,5%	0%	0%	0%

Source: MCTI (2021). 4º Inventário nacional de emissões.

With every increment of global warming, regional changes in mean climate and extremes become more widespread and pronounced

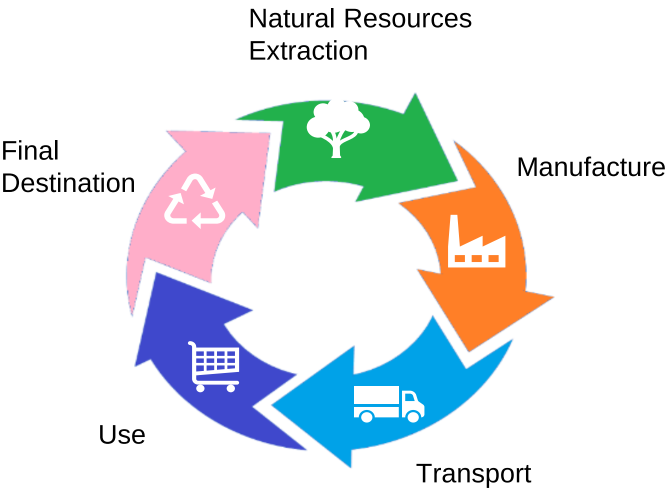


Source: IPCC AR6 (2023)

Life Cycle Assessment

Life Cycle Assessment (LCA):

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.



Source: ISO14040 (2006)

Life Cycle Assessment

Standardization - Life Cycle Assessment (LCA). :

- ISO 14040:2006 Environmental management -- Life cycle assessment -- Principles and framework. ISO 14040: 2006/Amd 1:2020 Environmental management – Life cycle assessment – Principles and framework – Amendment 1.
- ISO 14044:2006 Environmental management – Life cycle assessment – Requirements and guidelines.
- ISO 14044:2006/Amd 1:2017 Environmental management – Life cycle assessment – Requirements and guidelines. Amendment 1.
- ISO 14044:2006/Amd 2:2020 Environmental management – Life cycle assessment – Requirements and guidelines. Amendment 2.

Why should you make a LCA?

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

ECO FRIENDLY

Source: ISO14040 (2006)

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

Source: ISO14040 (2006)

Goal and Scope

Goal:

The goal has four key aspects ISO 14044 (2006)

- ✓ Intended Application of the study
- ✓ The purpose of the study
- ✓ The intended audience
- ✓ Use of comparative analysis

Example:

LCA Element	Summary for this Work
Intended Application	To compare the energy and environmental impact of LED lamps used in general illumination applications with traditional lighting products.
Reasons for the Study	• To quantify the energy and environment impacts of LEDs. • To address uncertainty in the existing body of literature and LCA reports concerning LED manufacturing methods and assumptions.
Audience	Lighting designers, policy makers, researchers and technical experts considering LED technology in general illumination applications.
Public Results	Results of this study will be freely available, published on the U.S. DOE Solid State Lighting website: http://www1.eere.energy.gov/buildings/ssl/

Source:
US Department of Energy. Life-Cycle Assessment of Energy and Environmental Impacts of LED Lighting Products

Goal and Scope

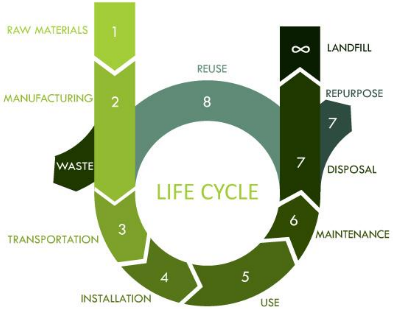
Scope:

- ✓ System under study (description of the system)
- ✓ System boundaries
- ✓ Function of the product and functional unit
- ✓ Allocation procedures
- ✓ Impact categories and the impact assessment method
- ✓ Data requirements
- ✓ …

Goal and Scope

System Boundaries:

- ✓ **Cradle to Grave:** 1-7
- ✓ **Cradle to Gate:** 1-2
- ✓ **Gate to Grave:** 3-7
- ✓ **Gate to Gate:** 2



Source:
Matssura et al. RenovaCalc

Example:

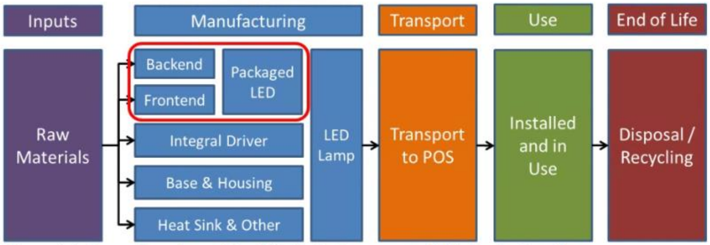


Figure 4-1. System boundary of the Life Cycle Assessment of this Study (Part 2)

-> Process Diagram is useful!

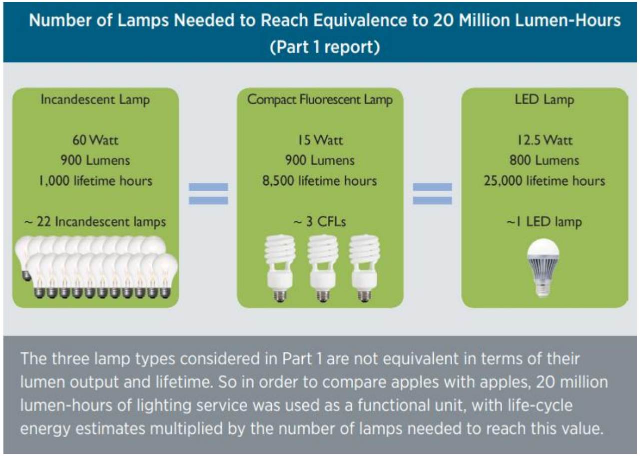
Source:
US Department of Energy. Life-Cycle Assessment of Energy and Environmental Impacts of LED Lighting Products

Goal and Scope

System function and functional unit:

- ✓ To describe a product the product's function has to be defined. The functional unit is the quantified definition of the function of a product.

Example:



Function:
Intensity of illumination over a lifetime

Functional unit: 20 million Lumen-Hours

Source:
US Department of Energy. Life-Cycle Assessment of Energy and Environmental Impacts of LED Lighting Products

Goal and Scope

Life Cycle Assessment Categories from CML-IA Methodology

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-dichlorobenzene)
EcoToxicity	Acute and chronic toxicity in ecosystems	1,4-dichlorobenzene, Mercury, Arsenic	kg 1,4-DB eq (1,4-dichlorobenzene)

Goal and Scope

In case of multi-product system:

- Expand the product system (consequential)

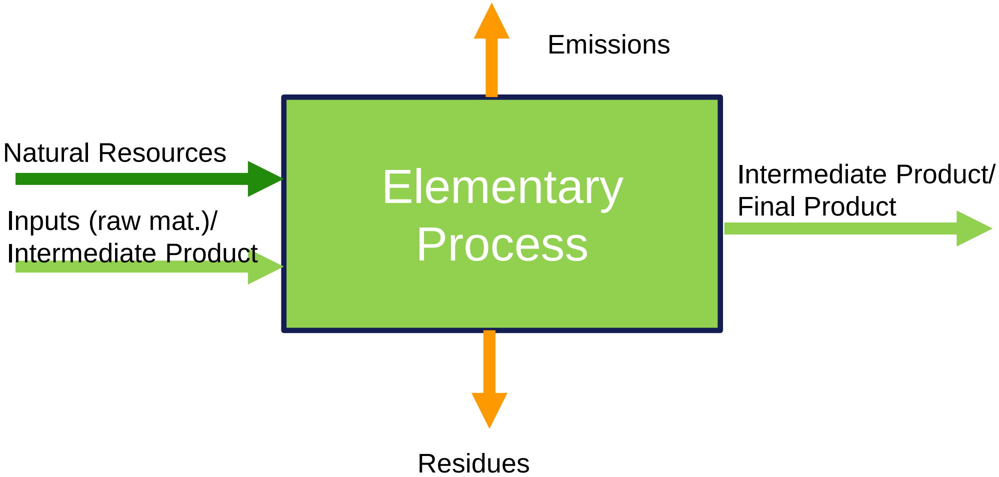
- Allocation of the impacts (attributional)

- **Allocation by Mass:** The inputs and outputs of a process are assigned to all of its products proportionally to their mass
- **Allocation by Energy:** The inputs and outputs of a process are assigned to all of its products according to their heating value. This allocation method is often used for production processes of fuels.
- **Allocation by Economic Value:** The inputs and outputs of a process are assigned to all of its products according to their market value.
- **Allocation by Other Rules:** This can include exergy, substance content, etc.

Source:
Adapted from Gabi. GaBi Paper Clip Tutorial

Life Cycle Assessment

Life Cycle Assessment Concepts
Elementary Process



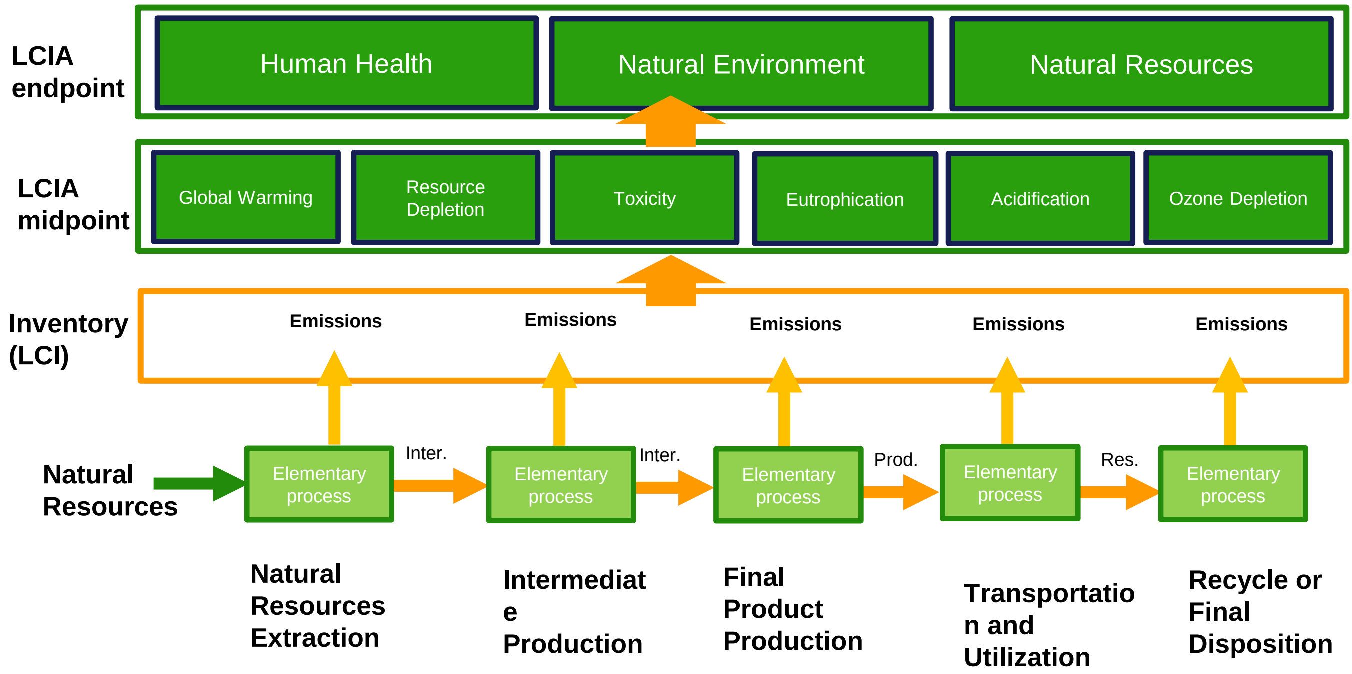
Example Carbon Capture Case Study Inventory[1]

Functional unit 1t CO2 captured

Flow	Category	Amount	Unit	Description
Inputs				
monoethanolamine	C:Manufacturing/2011:Manufacture of basic chemicals	5.28	kg	100%wt. MEA. MEA Makeup from Carbon Capture Unit
natural gas production | natural gas, energy based		6616872.40	kJ	Natural Gas of CHP
triethylene glycol	E:Water supply; sewerage, waste management and remediation activities	0.22	kg	99.5%. TEG Makeup from Carbon Capture Unit
water, decarbonised	E:Water supply; sewerage, waste management and remediation activities	3048.82	kg	Net Water Makeup from MEA and CWT units
Carbon dioxide	Elementary flows/Resource/in air	819.41	kg	CO2 input from Carbon Capture unit
Nitrogen	Elementary flows/Resource/in air	76600.62	kg	Air Input in CHP/ Air from input of CCU
Oxygen	Elementary flows/Resource/in air	21968.50	kg	Air Input in CHP/ Air from input of CCU
Water, in air	Elementary flows/Resource/in air	852.83	kg	Air Input in CHP/ Air from input of CCU
Outputs				
CO2 to wells - MEA Carbon Capture - TW		1000.00	kg	CO2 to the wells
electricity, medium voltage	D:Electricity, gas, steam and air conditioning supply	328812.65	kJ	Net Electricity Produced
Carbon dioxide, fossil	Elementary flows/Emission to air/unspecified	146.07	kg	from CC MEA unit, treated gas.
Carbon dioxide, fossil	Elementary flows/Emission to air/unspecified	35.99	kg	Others CO2 emissions
Monoethanolamine	Elementary flows/Emission to air/unspecified	5.26	kg	from CC MEA unit, treated gas
Nitrogen	Elementary flows/Emission to air/unspecified	9315.59	kg	Emission to Air
Oxygen	Elementary flows/Emission to air/unspecified	1009.39	kg	from Oxygen Removal Unit.
Water	Elementary flows/Emission to air/unspecified	1218.03	kg	Emission to Air

[1] Based on Aspen Hysys Simulation Results.

Life Cycle Assessment



EMSO_OLCA

processes

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Simultaneous Life Cycle Assessment and Process Simulation for Sustainable Process Design

by **Simone C. Miyoshi** and **Argimiro R. Secchi** *

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(This article belongs to the Special Issue **Modeling, Simulation, Control, and Optimization of Processes**)

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EMSO_OLCA

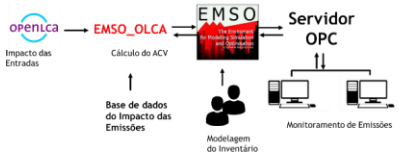
EMSO:

- **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**,...
- **Update** 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**

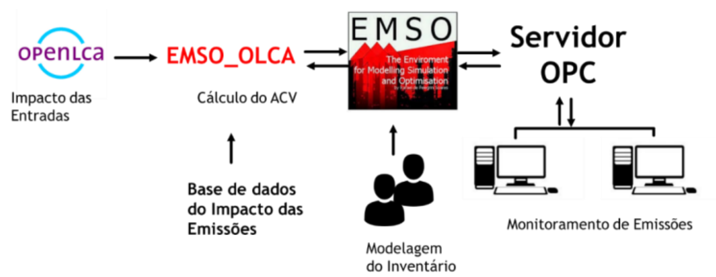
- ✓ **OpenLCA Impact Methodologies Available**:
  - ✓ 99 methodologies: IPCC, 2013; CML, 2001; ReCiPe, 2016; ...
  - ✓ 1479 Characterization Factors

- ✓ **OpenLCA** database update

EMSO_OLCA

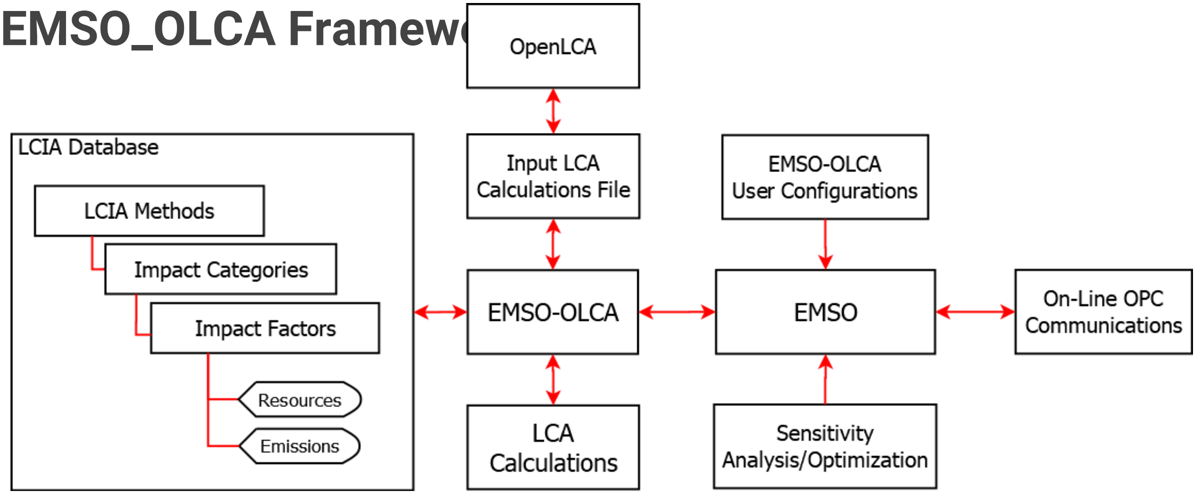
Applications:

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



EMSO_OLCA

EMSO_OLCA Framew



EMSO_OLCA

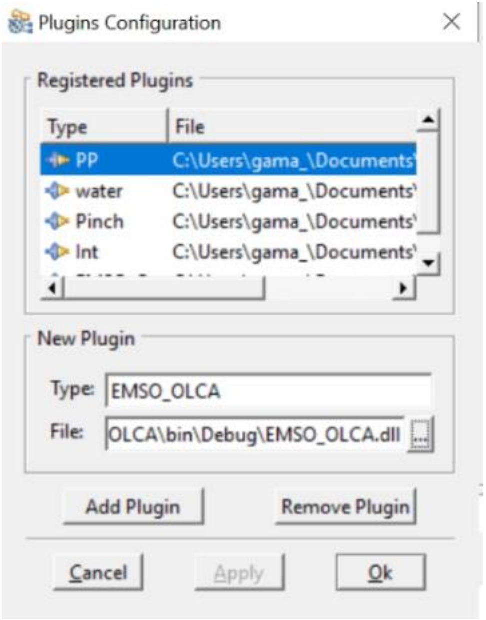
Installation

- 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.

Identification of the Emissions Flows Example: Co-generation Steam and Electricity

Inventory
Inputs
Bagasse/Straw
Water

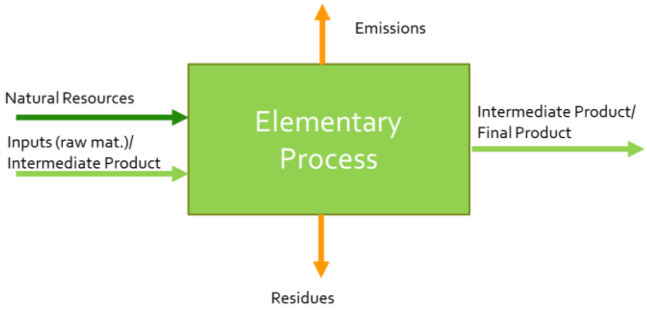
Inputs

Emissions
VOC
CO
NO
Particulate M., < 2,5 um
Particulate M., < 10um
SO
BC
OC
CH_4
N_2O
CO_2, biogenic

Emissions from process (Elementary Flows)

Products
Vapor
Bioelectricity, net

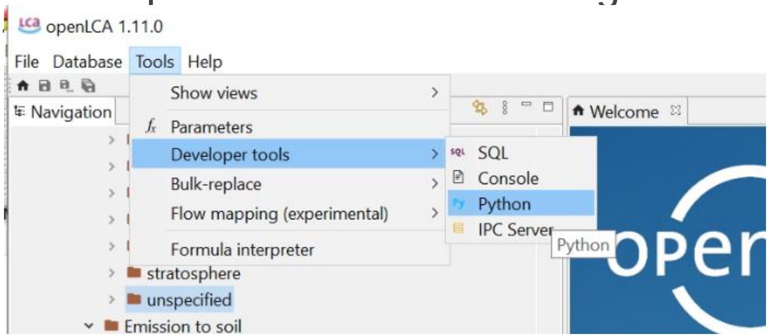
Outputs:
Multi-Product System



EMSO_OLCA

Get Impact Assessment from Inputs -> Input LCA File

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



EMSO_OLCA

Input LCA File

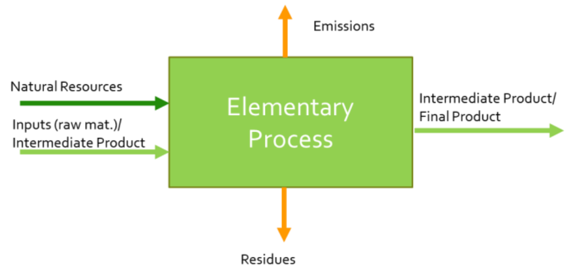
To export the entries in a .csv file, please:

- ✓ 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

natural resources,
emissions or
waste.



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=[“Path/methods_database”],
MethodName= ["MethodName"],
ImpactCategory=["ImpactCategory1", " ImpactCategory2"],
InputFileName=[“Path/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=[“Path/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
```

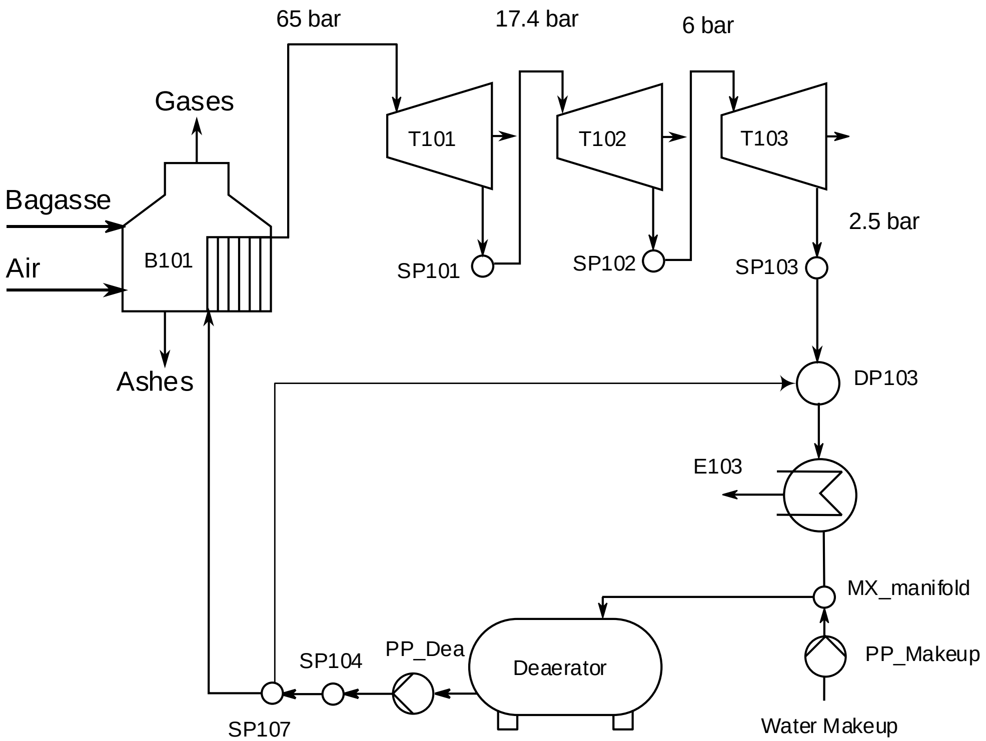
EMSO_OLCA Test

Ethanol Test Case - EcoInvent 3.8, ethanol production autonomous plant, BR, 1Kg
CML Baseline

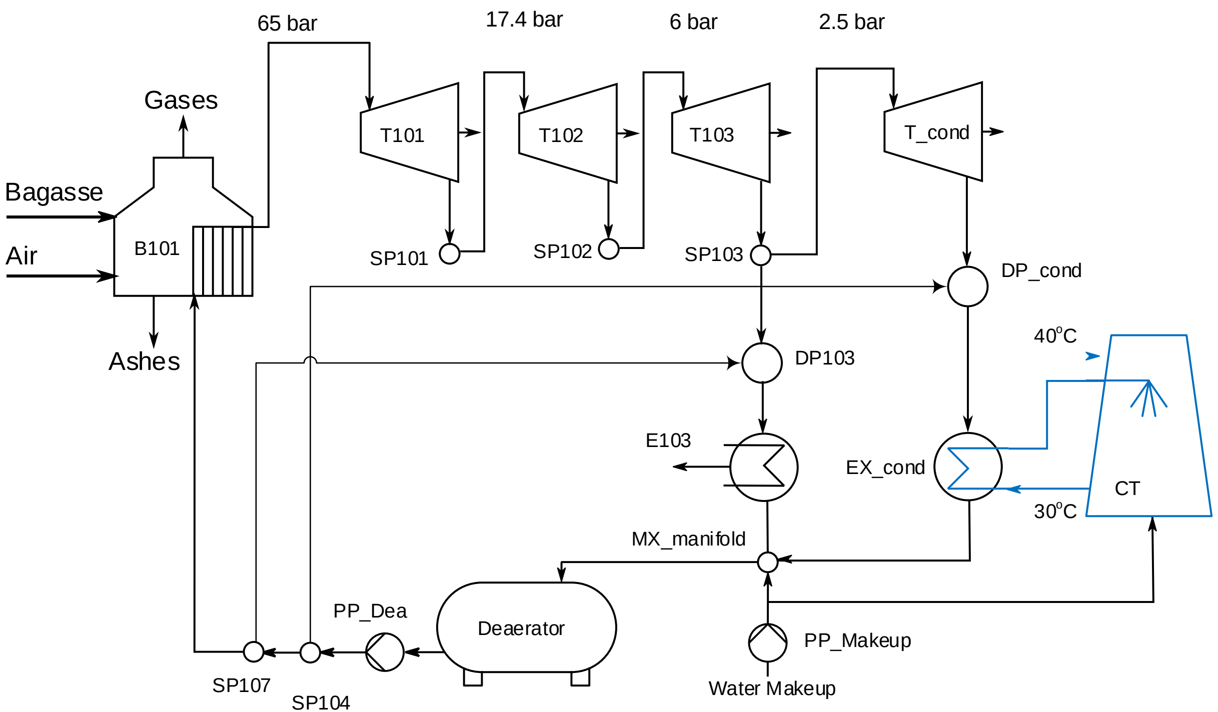
Impact category	Reference unit	OpenLCA Result	OLCA_EMSO Result	% Error
Abiotic depletion	kg Sb eq	$4.2916 \cdot 10^{-6}$	$4.2962 \cdot 10^{-6}$	0.1083%
Abiotic depletion (fossil fuels)	MJ	3.2862	3.2862	-0.0001%
Acidification	kg SO2 eq	$1.3946 \cdot 10^{-2}$	$1.3946 \cdot 10^{-2}$	0.0001%
Eutrophication	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%

Bioelectricity and Steam Co-generation
Scenario 1 – without condensing turbine



Bioelectricity and Steam Co-generation
Scenario2 -with condensing turbine



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)

Cogeneration Analysis
Inventory Results

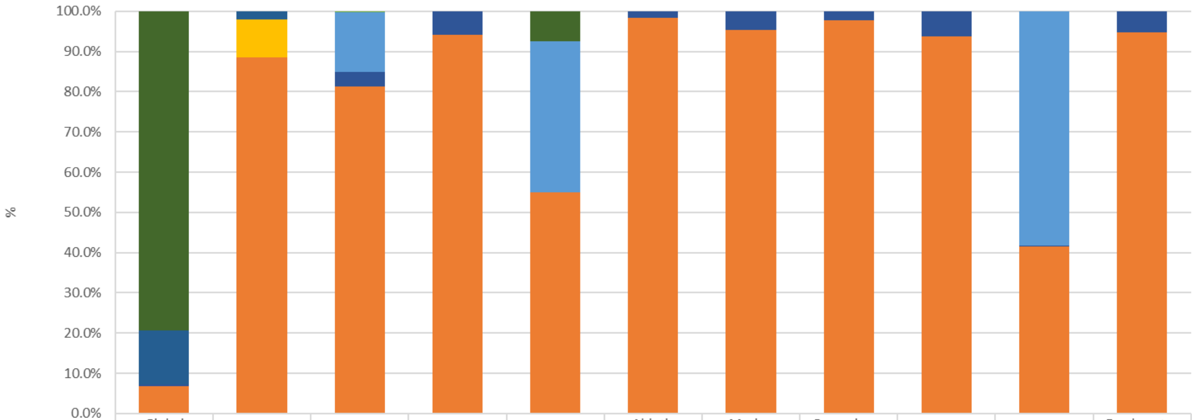
Inventory	Unit	Scenario 1	Scenario 2	Δ%
Inputs				
Bagasse/Straw	t/h	38.04	129.06	239%
Water	t/h	7.46	479.56	6333%
Emissions				
VOC	kg/h	0.32	1.08	239%
CO	kg/h	5.06	17.18	239%
NO	kg/h	33.34	113.11	239%
Particulate M., < 2,5 um	kg/h	0.66	2.23	239%
Particulate M., < 10um	kg/h	0.74	2.53	239%
SO	kg/h	30.59	103.79	239%
BC	kg/h	0.09	0.31	239%
OC	kg/h	0.21	0.73	239%
CH_4	kg/h	5.12	17.38	239%
N_2O	kg/h	3.17	10.76	239%
CO_2, biogenic	t/h	61.56	208.87	239%
Products				
Vapor	MWh	113.50	113.50	0%
Bioelectricity, net	MWh	34.02	154.38	354%

Cogeneration Analysis
LCA Results

Impact Category	Unit	Scenario 1	Scenario 2	Δ%
Global Warming (GWP100a)	kg CO_2 eq/MJ	$1.995 \cdot 10^{-3}$	$4.033 \cdot 10^{-3}$	102%
Photochemical oxidation	kg C_2H_4 eq/MJ	$2.761 \cdot 10^{-6}$	$5.285 \cdot 10^{-6}$	91%
Human toxicity	kg 1,4-DB eq/MJ	$5.087 \cdot 10^{-4}$	$1.571 \cdot 10^{-3}$	209%
Abiotic depletion	kg Sb eq/MJ	$7.270 \cdot 10^{-9}$	$2.776 \cdot 10^{-8}$	282%
Eutrophication	kg PO_4-eq/MJ	$2.172 \cdot 10^{-5}$	$4.120 \cdot 10^{-5}$	90%
Abiotic depletion (fossil fuels)	MJ/MJ	$5.979 \cdot 10^{-3}$	$1.448 \cdot 10^{-2}$	142%
Marine aquatic ecotoxicity	kg 1,4-DB eq/MJ	$4.470 \cdot 10^{-1}$	1.533E+00	243%
Ozone layer depletion (ODP)	kg CFC-11 – eq/MJ	$3.558 \cdot 10^{-11}$	9.244E-11	160%
Terrestrial ecotoxicity	kg 1,4-DB eq/MJ	$1.955 \cdot 10^{-6}$	7.737E-06	296%
Acidification	kg SO_2-eq/MJ	$5.381 \cdot 10^{-5}$	1.026E-04	91%
Fresh water aquatic ecotox.	kg 1,4-DB eq/MJ	$2.411 \cdot 10^{-4}$	8.787E-04	264%

Cogeneration Analysis

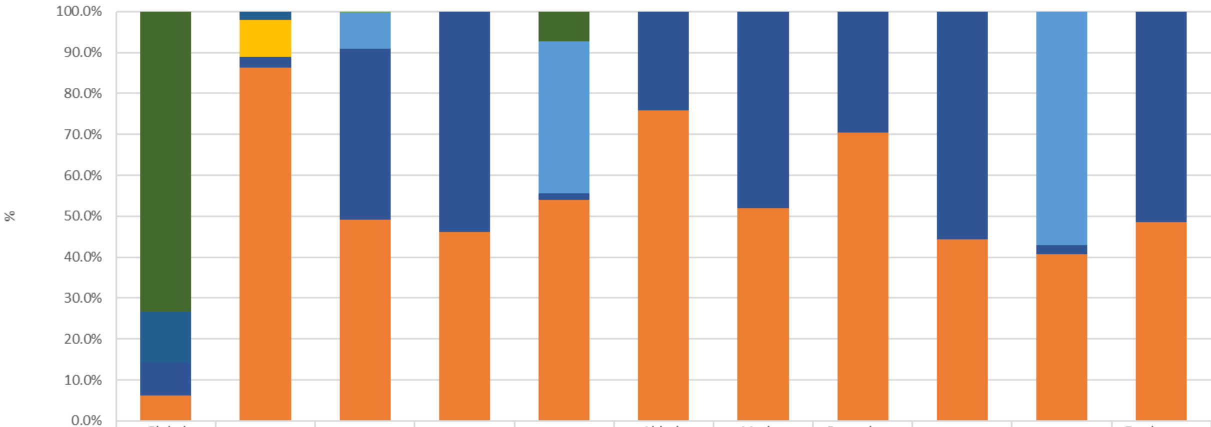
Contribution of Inputs and Emissions on Result – Scenari



	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%

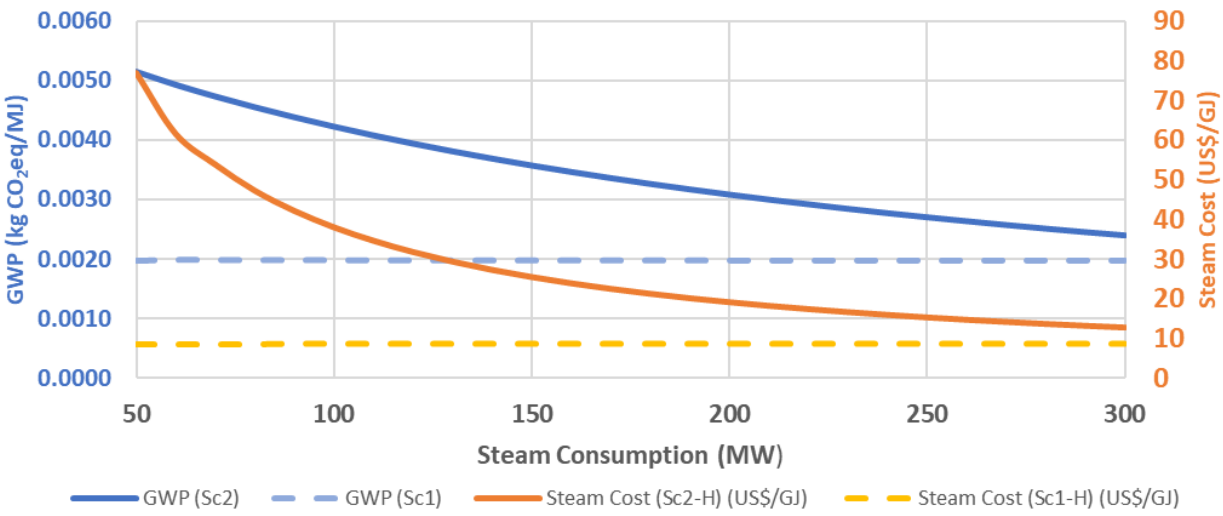
Cogeneration Analysis

Contribution of Inputs and Emissions on Result – Scenari



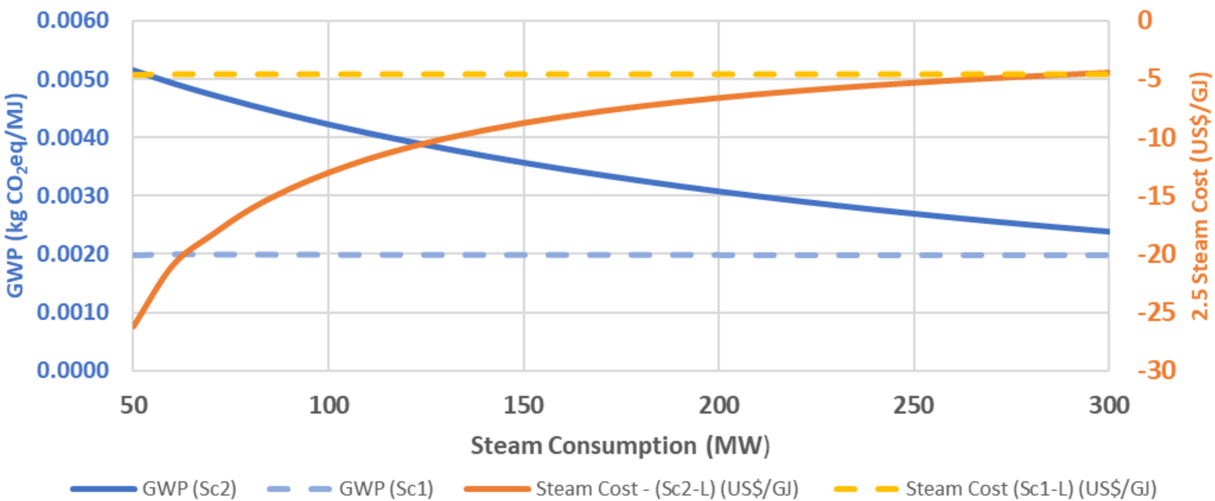
	Global warming (GWP100a)	Photochemical oxidation	Human toxicity	Abiotic depletion	Eutrophication	Abiotic depletion (fossil fuels)	Marine aquatic ecotoxicity	Ozone layer depletion (ODP)	Terrestrial ecotoxicity	Acidification	Fresh water aquatic ecotox.
CO2, Biogenic	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	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 Analysis
Results
Effect on GWP and Steam Cost, varying Steam Consumptio



High Bagasse Price: 0.150 US$/kg

Cogeneration Analysis
Results
Effect on GWP and Steam Cost, varying Steam Consumptio



Low Bagasse Price: 0.015 US$/kg

Examples - Bottle

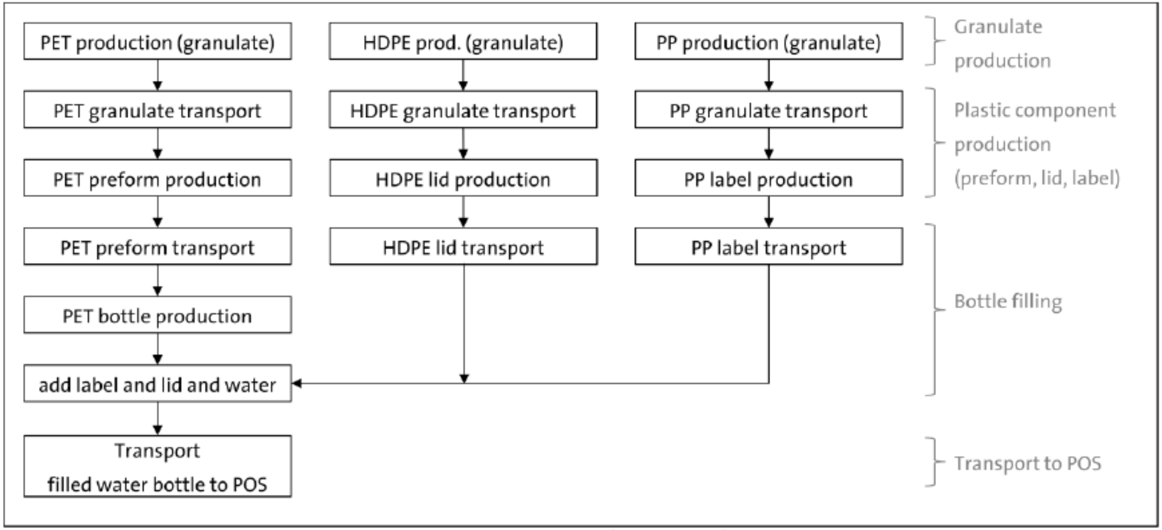
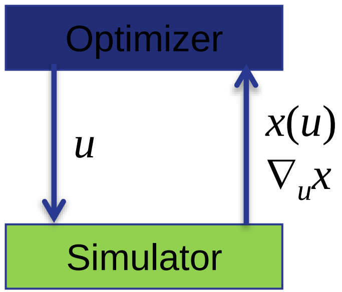


Figure 2: System boundaries, edited from Papong (2014, 541). PET = polyethylene terephthalate, PP = polypropylene, HDPE = high density polyethylene, POS = point of sale

Cogeneration Analysis
Results
Minimize vapor price varying condenser duty (u)

Feasible path approach

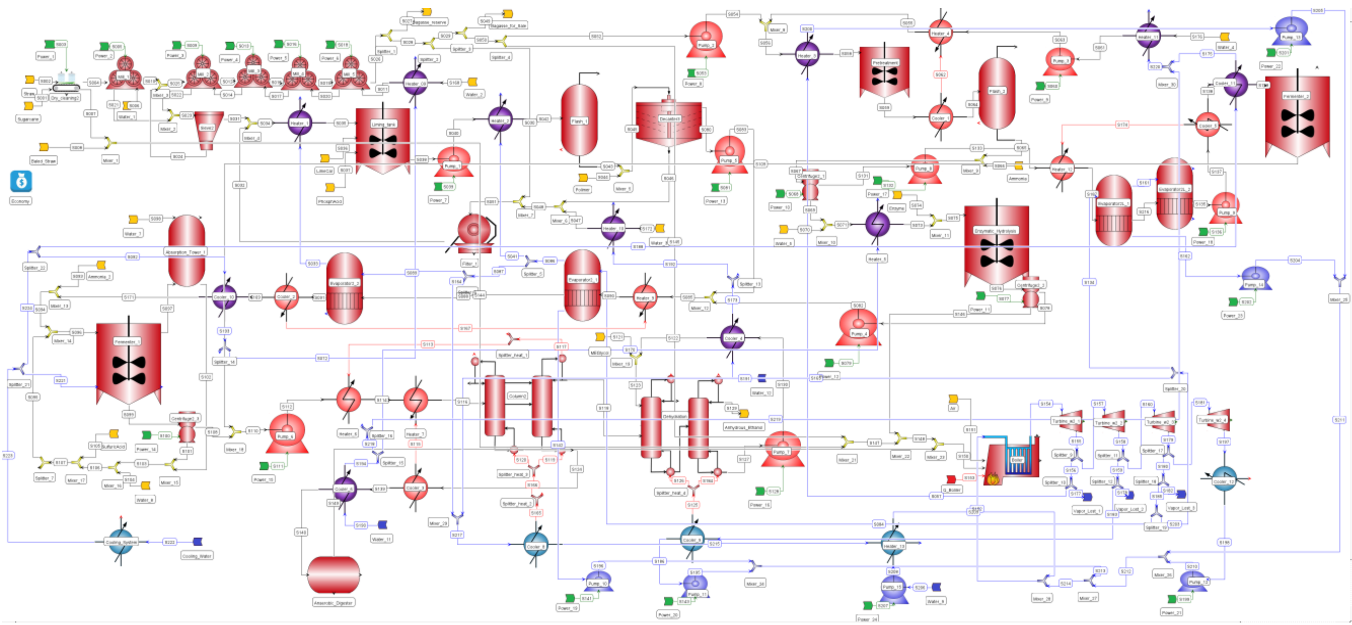


$$\min \; Vapor\ Price$$
s.t.:
$$x(u) \in \{x \in X \subseteq \Re^m \,/\, h(x,u) = 0\}$$

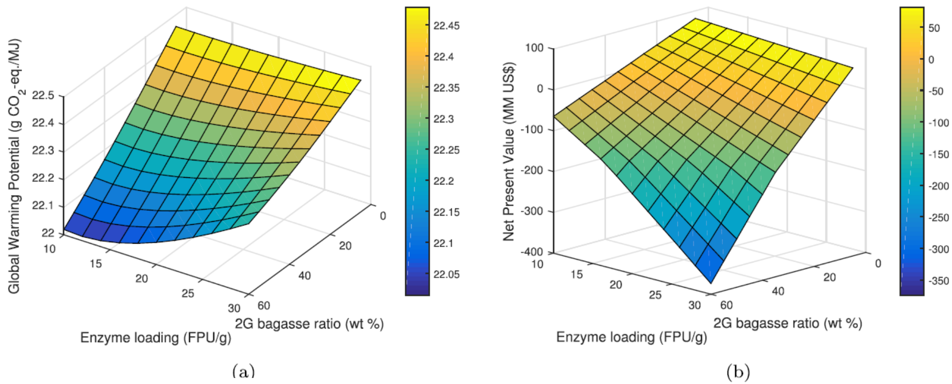
$$\nabla_u x = -\nabla_u h \, [\nabla_x h]^{-1} \qquad J^T(x,u) = \nabla_x h$$

Ethanol 1G-2G

Process Flow Diagram in EMSO



Ethanol 1G-2G



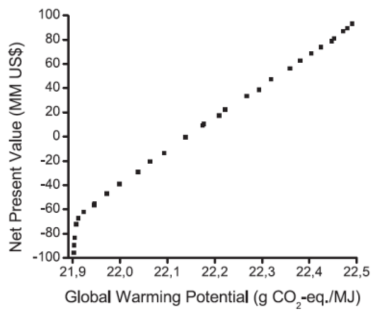


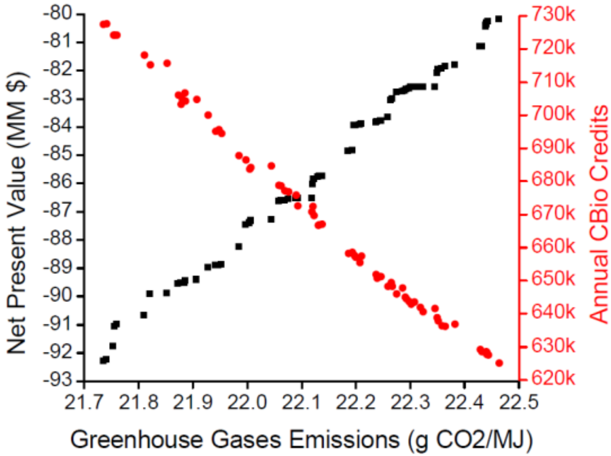
Fig. 3. Pareto set of optimal results for Net Present Value and Global Warming Potential.

Multi-objective optimization
- 2G bagasse ratio
- Solid loading
- Enzyme loading

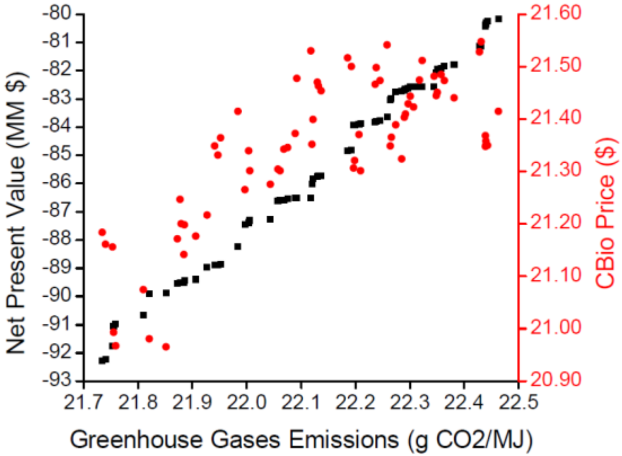
Source: Carpio et al (2021). *J.Clean. Prod.*

Ethanol 1G-2G

Pareto set of optimal solutions

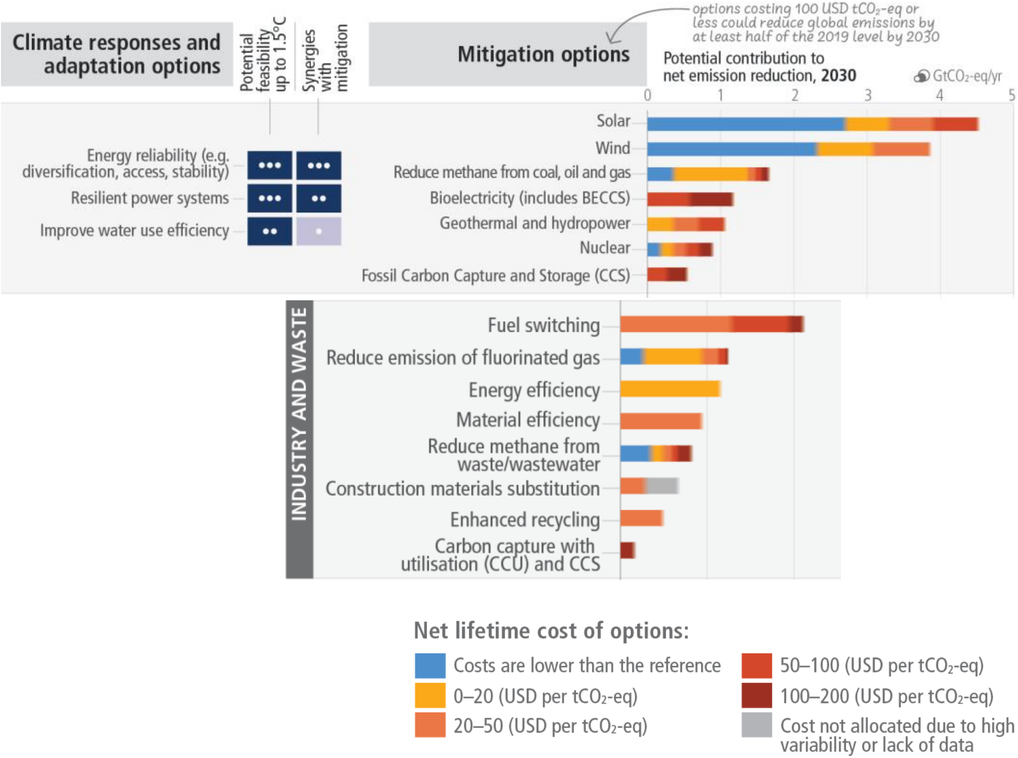


The integrated biorefinery would award about 625-728 mil CBio credits yearly.



The CBio price to achieve economic feasibility of the integrated biorefinery would be about \$20.96-\$21.55.

Opportunities in ChemEng



Source: IPCC AR6 (2023)