Outline of Part 3

Objective: Cover the basic principles of Systems Modeling for a Renewable Energy Process and be able to model a simple system.

- Importance of Systems Modeling in Renewable Energy
- Modeling systems
  - Stream properties
  - Thermodynamic relationships
  - Unit models
- Heat integration & Pinch Analysis
  - Basic Principles
  - Composite Curves
  - The Heat Cascade and the Grand Composite Curve
- **Life Cycle Assessment**
  - Goal & Scope Definition
  - Life Cycle Inventory
  - Life Cycle Impact Assessment
- Uncertainty Analysis & The Monte Carlo Method

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Life Cycle Assessment

With process modeling and energy integration, we can quantify matter flows, economics or efficiency.

What about sustainability?

This is a complex question… It depends on the precise definition of the product, process and the question.

For example:

Is an electric car more sustainable gasoline-powered car?

Probably… but what if the electricity comes from a gas-fired power plant? What if the battery needs to be replaced every 3 years?

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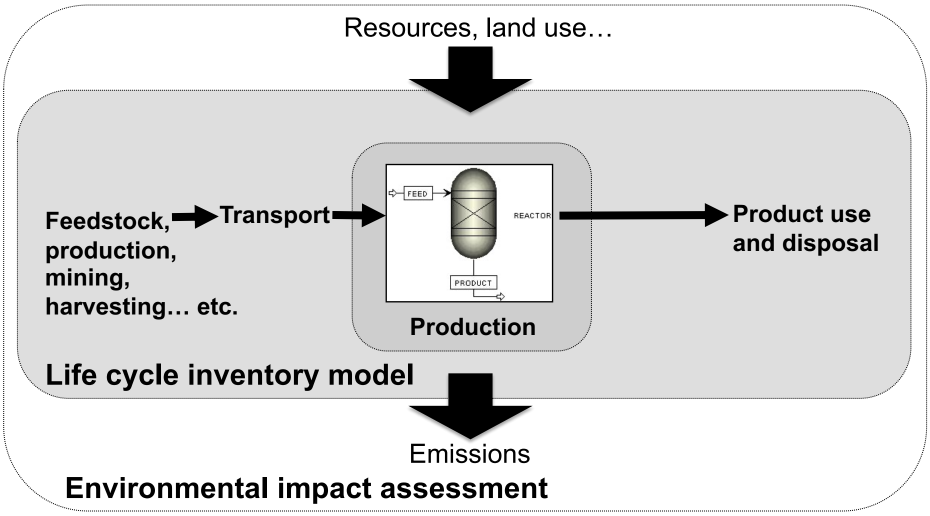
Life Cycle Assessment

Recall our general systems modeling approach:



This is a cradle-to-grave model.

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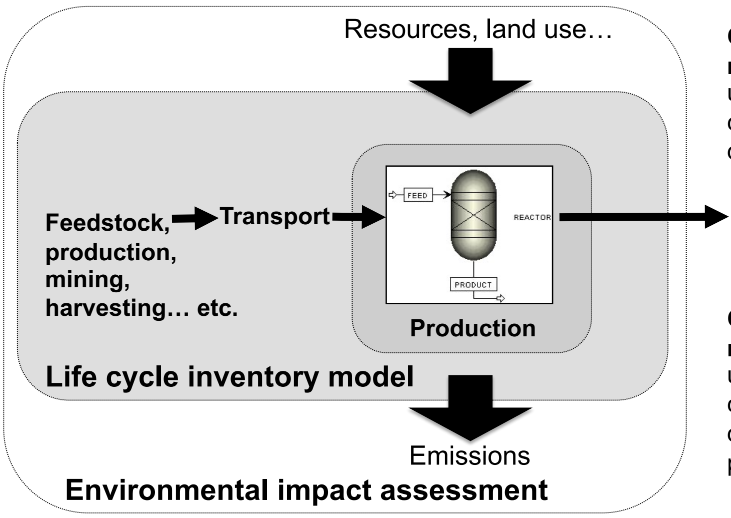
Life Cycle Assessment

Recall our general systems modeling approach:



Cradle-to-grave models are usually used for comparing different products.

Cradle-to-gate models are usually used for comparing different processes.

This is a cradle-to-gate model.

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Life Cycle Assessment

Life cycle assessment is usually performed in three phases:

1. Goal and Scope Definition → This is done before modeling
2. Life Cycle Inventory → This is the bulk of the modeling
3. Life Cycle Impact Assessment → This links modeling input-outputs with environmental impact models

Let's look at these steps in order…

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Life Cycle Assessment

Goal and Scope Definition

This is where various aspects of your model are defined…

A good place to start is by defining a *functional unit* (=product quantity or action that will normalize the results)

Examples of functional units:

1 MW of CH_4 produced globally

1 km driven in Switzerland

1 car used for it's entire lifetime

…

→ Functional units often define scope and boundaries:

- Geographical boundaries
- Use boundaries (gate or grave)
- Assumptions
- …

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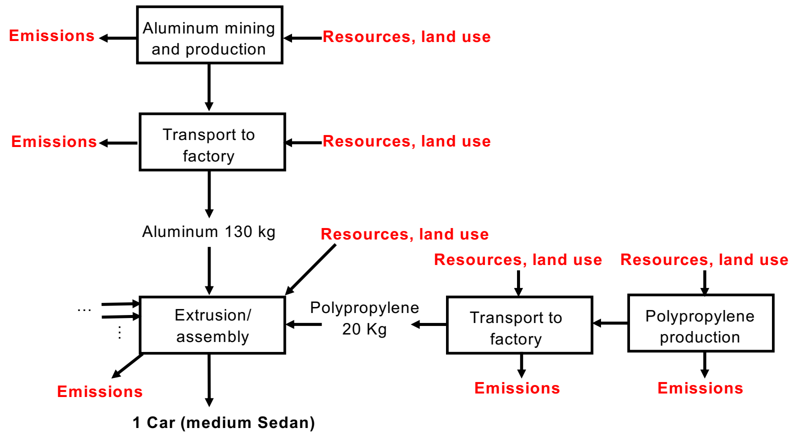
Life Cycle Assessment

Life Cycle Inventory

This is the modeling phase.

Let's look at an example:



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Life Cycle Assessment

Life Cycle Inventory

This is the modeling phase.

Let's look at an example:

These are activities.

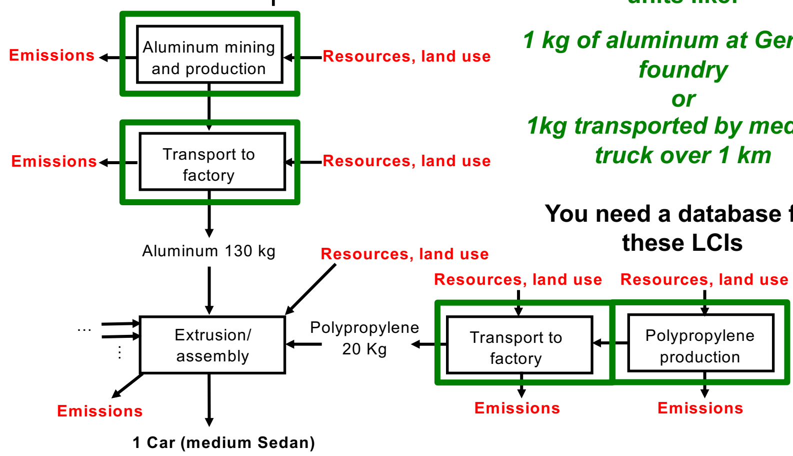
They are generally the results of other LCIs with functional units like:

1 kg of aluminum at German foundry

or

1kg transported by medium truck over 1 km

You need a database for these LCIs



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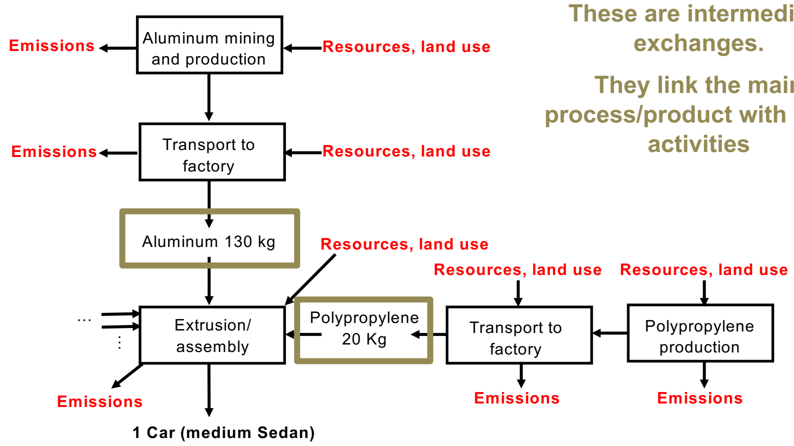
Life Cycle Assessment

Life Cycle Inventory

This is the modeling phase.

Let's look at an example:



These are intermediate exchanges.

They link the main process/product with other activities

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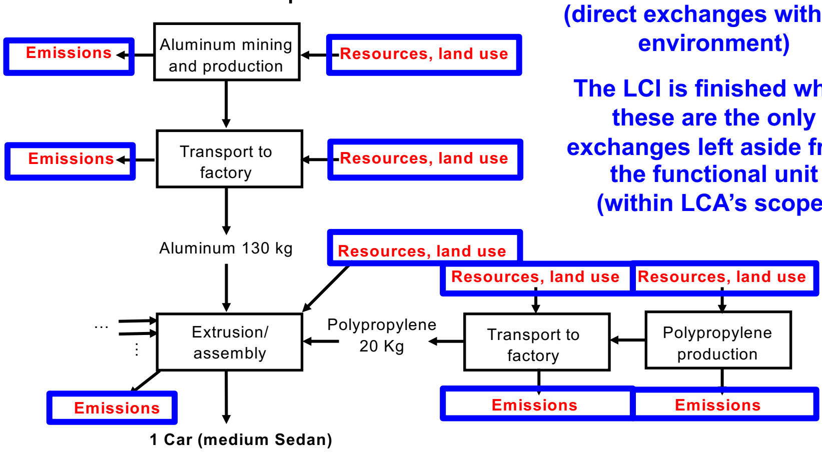
Life Cycle Assessment

Life Cycle Inventory

This is the modeling phase.

Let's look at an example:



These are elementary exchanges

(direct exchanges with the environment)

The LCI is finished when these are the only exchanges left aside from the functional unit (within LCA's scope)

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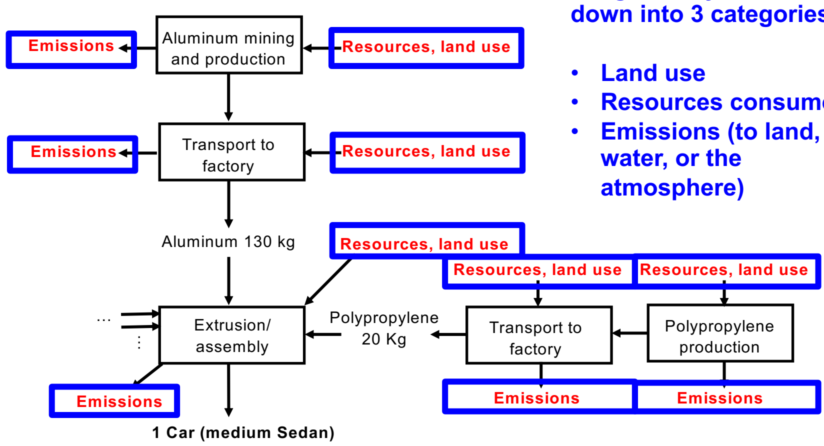
Life Cycle Assessment

Life Cycle Inventory

This is the modeling phase.

Let's look at an example:



Elementary exchanges are generally broken down into 3 categories:

- **Land use**
- **Resources consumed**
- **Emissions (to land, water, or the atmosphere)**

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Life Cycle Assessment

Life Cycle Inventory

For the LCI, you need a database a database of activities. One of the better known databases is called Ecoinvent and was based on a Swiss Startup.

List of activities

1	activity uuid	activityName	geography	start date	end date	ISIC number	ISIC class	specialActivityType
2	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
3	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
4	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
5	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
6	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
7	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
8	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
9	00093951-0c71-4a74-96d8-ece56003838a	treatment of used laptop computer, manual dismantling	CH	2005-01-01	2005-12-31	3830	Materials recovery	ordinary transforming activity
10	000b493f-5e76-4fe0-93ca-73b49263c1fc	chlorine dioxide production	GLO	2000-01-01	2000-12-31	2011	Manufacture of basic chemicals	ordinary transforming activity
11	001a7c31-a39b-4606-9877-d6cfc36e5fd8	polyurethane production, rigid foam	RER	1997-01-01	1997-12-31	2013	Manufacture of plastics and synth	ordinary transforming activity
12	001a7c31-a39b-4606-9877-d6cfc36e5fd8	polyurethane production, rigid foam	RER	1997-01-01	1997-12-31	2013	Manufacture of plastics and synth	ordinary transforming activity
13	001b83bb-d07c-4c91-90c1-5a9437badf06	2-nitroaniline production	GLO	2010-01-01	2010-12-31	2011	Manufacture of basic chemicals	ordinary transforming activity
14	001fa547-fbbd-4172-9492-0f58076c4553	market for used locomotive	GLO	2011-01-01	2011-12-31	3830	Materials recovery	market activity
15	002da2f2-595b-427e-ae3a-3f7dcd769715	softwood forestry, mixed species, sustainable forest manag	GLO	2010-01-01	2012-12-31	0220	Logging	ordinary transforming activity
16	002da2f2-595b-427e-ae3a-3f7dcd769715	softwood forestry, mixed species, sustainable forest manag	GLO	2010-01-01	2012-12-31	0220	Logging	ordinary transforming activity
17	002da2f2-595b-427e-ae3a-3f7dcd769715	softwood forestry, mixed species, sustainable forest manag	GLO	2010-01-01	2012-12-31	0220	Logging	ordinary transforming activity
18	002da2f2-595b-427e-ae3a-3f7dcd769715	softwood forestry, mixed species, sustainable forest manag	GLO	2010-01-01	2012-12-31	0220	Logging	ordinary transforming activity
19	002f9105-f892-4241-9c45-b3b7d68a9c72	power saw production, without catalytic converter	RER	1995-01-01	2001-12-31	2818	Manufacture of power-driven hand	ordinary transforming activity
20	00352317-8629-4778-96a7-abfa11c1face	treatment of waste polyethylene terephtalate, municipal i	GLO	2006-01-01	2012-12-31	3821	Treatment and disposal of non-ha	ordinary transforming activity
21	00352317-8629-4778-96a7-abfa11c1face	treatment of waste polyethylene terephtalate, municipal i	GLO	2006-01-01	2012-12-31	3821	Treatment and disposal of non-ha	ordinary transforming activity
22	00352317-8629-4778-96a7-abfa11c1face	treatment of waste polyethylene terephtalate, municipal i	GLO	2006-01-01	2012-12-31	3821	Treatment and disposal of non-ha	ordinary transforming activity
23	00352317-8629-4778-96a7-abfa11c1face	treatment of waste polyethylene terephtalate, municipal i	GLO	2006-01-01	2012-12-31	3821	Treatment and disposal of non-ha	ordinary transforming activity
24	0036e50d-8e5b-438c-b94c-4ee40350362b	electricity production, natural gas, conventional power pla	CN-HU	1990-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
25	0036e50d-8e5b-438c-b94c-4ee40350362b	electricity production, natural gas, conventional power pla	CN-HU	1990-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
26	003ad59e-1069-4a8f-ada1-6785cf19e74b	market for wastewater from medium density board product	GLO	2012-01-01	2012-12-31	3700	Sewerage	market activity
27	003b13f0-18f4-467d-91a6-4201072dadaa	market for electricity, medium voltage	CA-YK	2012-01-01	2015-12-31	3510	Electric power generation, transm	market activity
28	003e869a-f532-46cc-b8d4-641988008e6d	lath, hardwood, raw, air drying to u=20%	CA-QC	2011-01-01	2013-12-31	1610	Sawmilling and planing of wood	ordinary transforming activity
29	003f9a31-c540-4351-a434-3b1b1c791b99	electricity production, hard coal	NL	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
30	003f9a31-c540-4351-a434-3b1b1c791b99	electricity production, hard coal	NL	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
31	003f9a31-c540-4351-a434-3b1b1c791b99	electricity production, hard coal	NL	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
32	00420798-e9d1-4de9-8745-09bd85f31db8	treatment of blast furnace gas, in power plant	BR	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
33	00420798-e9d1-4de9-8745-09bd85f31db8	treatment of blast furnace gas, in power plant	BR	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity
34	00420798-e9d1-4de9-8745-09bd85f31db8	treatment of blast furnace gas, in power plant	BR	1980-01-01	2015-12-31	3510	Electric power generation, transm	ordinary transforming activity

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Life Cycle Assessment

Life Cycle Inventory

For the LCI, you need a database a database of activities. One of the better known databases is called Ecoinvent and was based on a Swiss Startup.

List of intermediate exchanges

1	name	unitName	CAS	synonyms	comment
2	kraft paper, unbleached	kg			
3	transport, passenger, motor scooter	person*km			
4	green manure, Swiss integrated production, until January	ha			
5	bentonite quarry infrastructure	unit			
6	integrated circuit, logic type	kg			
7	iron scrap, sorted, pressed	kg			
8	carboxymethyl cellulose, powder	kg	9000-11-7		
9	transport, freight, lorry 28 metric ton, vegetable oil methyl ester 100%	metric ton*km			
10	methane, 96% by volume, from biogas, high pressure, at user	MJ	000074-82-8		
11	bicycle	unit			
12	aircraft, medium haul	unit			
13	lithium	kg	7439-93-2		
14	aluminium removed by milling, average	kg			
15	polyurethane, flexible foam	kg	9009-54-5		
16	aluminium removed by turning, primarily roughing, computer numerical controlle	kg			
17	rye seed, for sowing	kg			
18	machine operation, diesel, < 18.64 kW, low load factor	hour			
19	sewer grid, 4.7E10l/year, 583 km	km			
20	lead smelter slag	kg			
21	concrete, 30-32MPa	m3			
22	furnace, wood chips, with silo, 50kW	unit			
23	impact extrusion of aluminium, 4 strokes	kg			
24	waste paperboard, sorted	kg			
25	cement, blast furnace slag 18-30% and 18-30% other alternative constituents	kg			
26	impact extrusion of aluminium, cold, initial surface treatment	kg			
27	benzal chloride	kg	98-87-3		
28	alfalfa-grass silage	kg			mix of alfalfa and thimothy ensiled for animal feed
29	diesel-electric generating set, 18.5kW	unit			
30	shale brick	kg			
31	used window frame, wood-metal	m2			
32	wastewater from grass refinery	m3			
33	potato starch	kg			

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Life Cycle Assessment

Life Cycle Inventory

For the LCI, you need a database a database of activities. One of the better known databases is called Ecoinvent and was based on a Swiss Startup.

List of elementary exchanges

	A	B	C	D	E	F
1	name	compar	subcompartment	unitName	casNumber	formula
155	Chlorsulfuron	soil	agricultural	kg	064902-72-3	
156	Choline chloride	soil	agricultural	kg	000067-48-1	
157	Chromium	air	urban air close to grour	kg	007440-47-3	
158	Chromium VI	air	urban air close to grour	kg	018540-29-9	
159	Chromium, 25.5% in chromite, 11.6% in crude ore,	natural re:	in ground	kg	007440-47-3	
160	Chromium, ion	water	ground-	kg	016065-83-1	
161	Chromium-51	air	urban air close to grour	kBq		
162	Chrysotile, in ground	natural re:	in ground	kg		
163	Cinidon-ethyl	soil	agricultural	kg	142891-20-1	
164	Cinnabar, in ground	natural re:	in ground	kg		
165	Clay, bentonite, in ground	natural re:	in ground	kg	001302-78-9	
166	Clay, unspecified, in ground	natural re:	in ground	kg		
167	Clethodim	soil	agricultural	kg	099129-21-2	
168	Clodinafop-propargyl	soil	agricultural	kg	105512-06-9	
169	Clomazone	soil	agricultural	kg	081777-89-1	
170	Clopyralid	soil	agricultural	kg	001702-17-6	
171	Cloquintocet-mexyl	soil	agricultural	kg	099607-70-2	
172	Cloransulam-methyl	soil	agricultural	kg	147150-35-4	
173	Coal, brown, in ground	natural re:	in ground	kg		
174	Coal, hard, unspecified, in ground	natural re:	in ground	kg		
175	Cobalt	air	urban air close to grour	kg	007440-48-4	
176	Cobalt, in ground	natural re:	in ground	kg	007440-48-4	
177	Cobalt-57	air	urban air close to grour	kBq		
178	Cobalt-58	air	urban air close to grour	kBq		
179	Cobalt-60	air	urban air close to grour	kBq		
180	COD, Chemical Oxygen Demand	water	ground-	kg		
181	Colemanite, in ground	natural re:	in ground	kg		
182	Copper	air	urban air close to grour	kg	007440-50-8	
183	Copper, 0.52% in sulfide, Cu 0.27% and Mo 8.2E-3%	natural re:	in ground	kg	007440-50-8	
184	Copper, 0.59% in sulfide, Cu 0.22% and Mo 8.2E-3%	natural re:	in ground	kg	007440-50-8	
185	Copper, 0.97% in sulfide, Cu 0.36% and Mo 4.1E-2%	natural re:	in ground	kg	007440-50-8	
186	Copper, 0.99% in sulfide, Cu 0.36% and Mo 8.2E-3%	natural re:	in ground	kg	007440-50-8	
591	Occupation, traffic area, road network	natural re:	land	m2*year		
592	Occupation, unspecified	natural re:	land	m2*year		
593	Occupation, unspecified, natural (non-use)	natural re:	land	m2*year		

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Life Cycle Assessment

Life Cycle Impact Assessment

LCIA translates the elemental exchanges into 1 or several environmental impacts.

The difficulty: How do you compare very different exchanges with the environment

For example:

1 kg of CO_2 emitted in the atmosphere (emission)

1 kg of aluminum ore extraction (resource)

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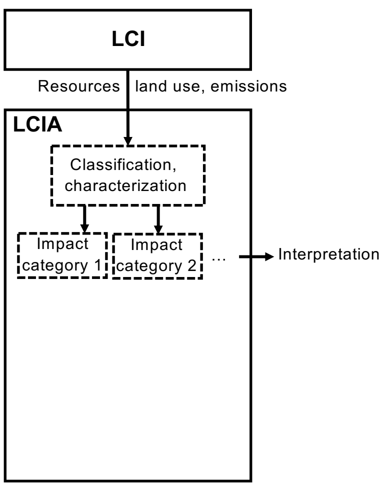
Life Cycle Assessment

Life Cycle Impact Assessment

The basic procedure:



1. Classification: Elementary exchange are grouped into impact categories
≈ physical phenomena (global warming potential or GWP, ecotoxicity…etc.)

2. Characterization: Calculation of the category impact from the exchanges classified in this category
We use *characterization factors* that are generally based on physical phenomena (e.g. radiative forcing values for GWP)

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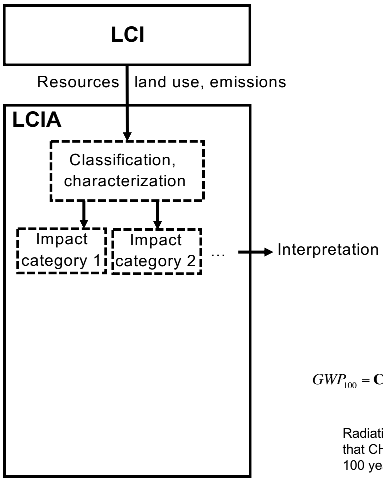
Life Cycle Assessment

Life Cycle Impact Assessment

The basic procedure:



Example of characterization and weighting:

You want to calculate the GWP_{100} from a list of elementary exchanges ***L****:*

$$\mathbf{L} = \begin{bmatrix} x\ kg\ CO_2\ emitted \\ y\ m^2\ land\ used \\ z\ kg\ CH_4\ emitted \\ \ldots \end{bmatrix}$$

Characterization and weighting would likely occur simultaneously using a single characterization vector ***C****:*

$$GWP_{100} = \mathbf{C}\,\mathbf{L} = \begin{bmatrix} 1 & 0 & 25 & \ldots \end{bmatrix} \begin{bmatrix} x\ kg\ CO_2\ emitted \\ y\ m^2\ land\ used \\ z\ kg\ CH_4\ emitted \\ \ldots \end{bmatrix} = x + 25z\ \text{ kg CO}_2\text{ equivalent}$$

Radiative forcing values show that CH_4 has 25x more GWP in 100 years than CO_2

Result is a single impact quantified in kg of CO_2 equivalent

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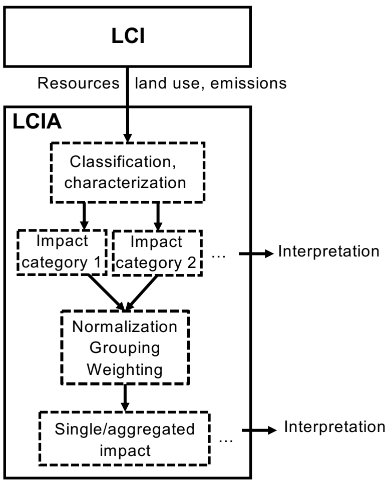
Life Cycle Assessment

Life Cycle Impact Assessment

The basic procedure:



3. Normalization/grouping /weighting: Category impacts are aggregated together into a single or several environmental impact indicators

These methods can be more or less rigorous (some are based on polling of experts). One of the more rigorous methods is based on calculating economic damages (how much multiple impacts will cost our economies).

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Outline of Part 2

Objective: Cover the basic principles of Systems Modeling for a Renewable Energy Process and be able to model a simple system.

- Importance of Systems Modeling in Renewable Energy
- Modeling systems
  - Stream properties
  - Thermodynamic relationships
  - Unit models
- Heat integration & Pinch Analysis
  - Basic Principles
  - Composite Curves
  - The Heat Cascade and the Grand Composite Curve
- Life Cycle Assessment
  - Goal & Scope Definition
  - Life Cycle Inventory
  - Life Cycle Impact Assessment
- **Uncertainty Analysis & The Monte Carlo Method**

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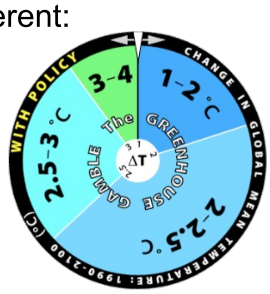
Uncertainty analysis

Uncertainty estimation **must** be a key part of systems modeling because predictions of complex systems are inherently uncertain.

These two predictions are very different:

The earth will warm by 2.1°C by 2100

Vs.



Uncertainty, can shape the conclusions!

Source: *MIT Global Change*

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Uncertainty analysis

You can often measure or estimate the uncertainty of your inputs or parameters (e.g. crop yields in a field, accuracy of a measured temperature, purity of a chemical…etc.).

How do you measure the effect on your model?

Through error propagation:

Analytically:

Dependent variable of interest e

$$\sigma_e^2 = \sum_i \left(\frac{\delta e}{\delta x_i} \right) \sigma_{x_i}^2$$

Cumulative variance of e (a function of variables x_i)

Independent variable x_i

Variance of x_i

However, for a complex system, there is no analytical function!

An alternative for such systems is the computational Monte Carlo Method…

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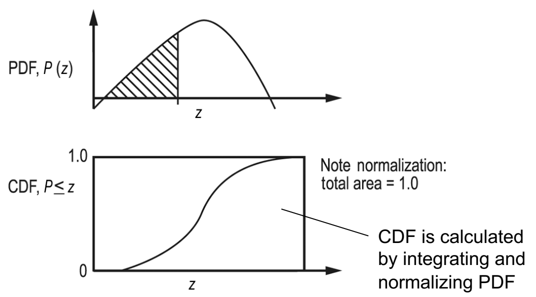
Monte Carlo Method

The Monte Carlo method is brute force method for calculating the unknown probability distribution of a dependent variable *e* from a set of known probability distributions of variables *z*.

This is ideal for complex system models!

It has 4 steps:

Step 1: Build a probability distribution function and cumulative probability distribution for each independent variable.



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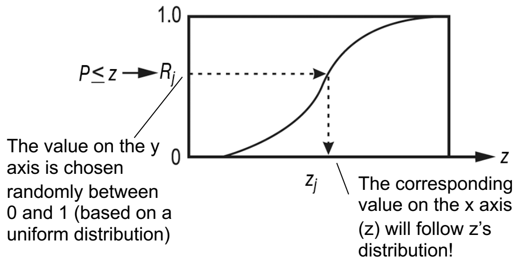
Monte Carlo Method

The Monte Carlo method is brute force method for calculating the unknown probability distribution of a dependent variable *e* from a set of known probability distributions of variables *z*.

This is ideal for complex system models!

It has 4 steps:

Step 2: The cumulative distribution function is used to generate a random value of each variable z that follows it's probability distribution.



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Monte Carlo Method

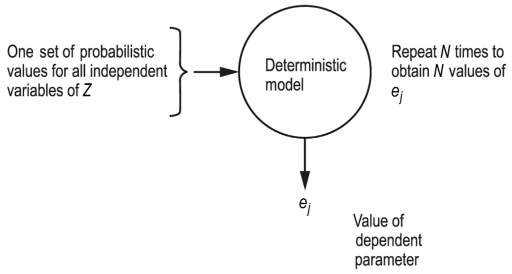
The Monte Carlo method is brute force method for calculating the unknown probability distribution of a dependent variable *e* from a set of known probability distributions of variables *z*.

This is ideal for complex system models!

It has 4 steps:

Step 3: Do this for all independent variables and calculate the dependent variable using your model

Do this many times!



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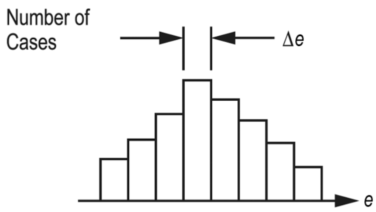
Monte Carlo Method

The Monte Carlo method is brute force method for calculating the unknown probability distribution of a dependent variable *e* from a set of known probability distributions of variables *z*.

This is ideal for complex system models!

It has 4 steps:

Step 4: Construct a probability distribution based on a histogram of your output data!



From this you can estimate the mean and variance of *e*:

$$\overline{e} = \frac{\sum_j e_j}{N} \qquad \sigma_e^2 = \frac{\sum_j (e_j - \overline{e})^2}{N(N-1)}$$

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Sustainable Energy Systems

3. Economic modeling

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Literature

- Smith, Robin M. *Chemical Process: Design and Integration*. New Jersey: John Wiley & Sons, 2005.
- Tester, Jefferson W. *Sustainable Energy: Choosing Among Options*. Cambridge, Mass: MIT Press, 2012.
- Sinnott, Ray, and Towler, Gavin. *Chemical Engineering Design*. Elsevier, 2020.

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Outline of Part 3

Objective: Introduce economic evaluation and the time value of money.

- Capital cost estimation
- Operating cost estimate
  - Typical operating costs
  - Externalities
- Time value of money
  - Continuous and discrete interest
  - Cash flows
  - Minimum selling price and rate of returns

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Capital cost estimation

Easiest method: using existing data

Accounting for capacity: This is where economies of scale come from….

Target capacity *Q*

Equipment-dependent exponent

$$C_{\mathrm{Q}} = C_{\mathrm{B}}\left(\frac{Q}{Q_B}\right)^{M}$$

Equipment cost at capacity *Q*

Equipment cost at base capacity

Base capacity

Values of M: 0.6, average across the industry (It's sometimes called the 6/10 rule)

0.8-0.9, Processes that use a lot of gas compression or mechanical handling (methanol plant, pulp and paper, etc.)

0.7, Petrochemical process

0.4-0.5, Highly instrumented process

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Capital cost estimation

Easiest method: using existing data

Accounting for capacity: This is where economies of scale come from….

Target capacity *Q*

Equipment-dependent exponent

$$C_{\mathrm{Q}} = C_{\mathrm{B}}\left(\frac{Q}{Q_B}\right)^{M}$$

Equipment cost at capacity *Q*

Equipment cost at base capacity

Base capacity

Correcting for the age of the data: Equipment costs evolve due to change inflation, change in materials, labor, etc.

Cost index in year *i*

$$C_i = C_j\left(\frac{Index_i}{Index_j}\right)$$

Equipment cost in year *i*

Equipment cost in year *j*

Cost index in year j

Common indexes: Chemical Engineering indexes, Mashall and Swift indexes (both published in *C&E News*), Nelson-Farrar Cost indexes are given in the *Oil and Gas Journal*.

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Capital cost estimation

(from a list of individual equipment)

Correction factors:

$$C_{\mathrm{Q,corr}} = C_{\mathrm{B}} \left(\frac{Q}{Q_B}\right)^M f_M f_P f_T$$

Design temperature correction

Material correction factor

Design pressure correction

Material	Correction factor f_M
Carbon steel	1.0
Aluminum	1.3
Stainless steel (low grades)	2.4
Stainless steel (high grades)	3.4
Hastelloy C	3.6
Monel	4.1
Nickel and inconel	4.4
Titanium	5.8

Design pressure (bar absolute)	Correction factor f_P
0.01	2.0
0.1	1.3
0.5 to 7	1.0
50	1.5
100	1.9

Design temperature (°C)	Correction factor f_T
0–100	1.0
300	1.6
500	2.1

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Capital cost estimation

(from a list of individual equipment)

Correction factors:

$$C_{\mathrm{Q}} = C_{\mathrm{B}} \left(\frac{Q}{Q_B}\right)^M f_M f_P f_T$$

Design temperature correction

Material correction factor

Design pressure correction

Installation costs:

$$C_{\mathrm{Total}} = \sum_i C_{Q,i} [f_M f_P f_T (1 + f_{PIP})]_i + \begin{pmatrix} f_{ER} + f_{INST} + f_{ELEC} + f_{UTIL} + f_{OS} \\ + f_{BUILD} + f_{SP} + f_{DEC} + f_{CONT} + f_{WC} \end{pmatrix} \sum_i C_{Q,i}$$

Item	Type of process	
	Fluid processing	Solid processing
Direct costs		
Equipment delivered cost	1	1
Equipment erection, f_{ER}	0.4	0.5
Piping (installed), f_{PIP}	0.7	0.2
Instrumentation & controls (installed), f_{INST}	0.2	0.1
Electrical (installed), f_{ELEC}	0.1	0.1
Utilities, f_{UTIL}	0.5	0.2
Off-sites, f_{OS}	0.2	0.2
Buildings (including services), f_{BUILD}	0.2	0.3
Site preparation, f_{SP}	0.1	0.1
Total capital cost of installed equipment	3.4	2.7
Indirect costs		
Design, engineering and construction, f_{DEC}	1.0	0.8
Contingency (about 10% of fixed capital costs), f_{CONT}	0.4	0.3
Total fixed capital cost	4.8	3.8
Working capital		
Working capital (15% of total capital cost), f_{WC}	0.7	0.6
Total capital cost, f_I	5.8	4.4

Working capital: reserve for start-up, raw material and product inventory, cash on hand, gap between receiving materials and selling products, spare parts... etc.

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Operating cost estimation

Typical costs:

Raw materials costs (RM) (chemicals, catalysts, etc…)

Costs from Chemical Marketing reporter, European chemical News, Asia Chemical News, Alibaba.com (The last one is free! But use large quantity offers).
→ All of these costs are variable and fluctuate with the market!

Utilities costs (U) (fuel, electricity, steam, cooling water, refrigeration, compressed air…etc.)

- Electricity and fuel costs tend to be available on public markets.
- Cooling water is fairly cheap and can usually be neglected (but is not free).
- Refrigeration, steam or compressed air can be produced in house or at least modeled as such…

Taxes (T): they are levied on gross profits (P) after allowances (i.e. deductions D) have been subtracted:

$$T = (P - D)t_R$$

Tax rate

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Operating cost estimation

Typical costs:

Operating labor costs (L):

Other fixed costs:

$Supervision \approx 0.25\ L$

$Overhead \approx 0.5\ (L + supervision)$

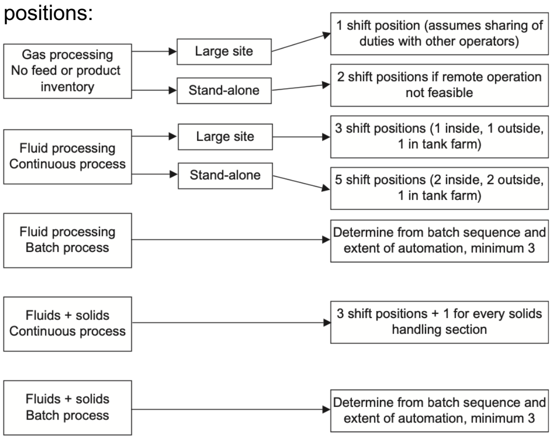
$Maintenance \approx 0.02\ C_{\text{Total}}$

$Rent\ of\ land \approx 0.02\ C_{\text{Total}}$

$Plant\ overhead^{*} \approx 0.65\ (L + supervision + overhead) + maintenance$

*This includes, HR, R&D, IT, finance, legal, etc…

Quick estimate of minimum number of shift positions:



1 operator will cost you 60’000 € / year or more

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Externalities

Externalities in the context of building a technology are an indirect cost or benefit to an uninvolved third party.

In the context of energy, they are often used to refer to the cost of environmental damages caused by the technology (i.e. a negative externality).

Two ways of dealing with them:

- Pay for the damages (after implementation)

  e.g. $SF\text{: } annualized\ contribution\ to\ decommissioning\ or\ a\ clean\text{–}up\ superfund$

- Impose an upfront tax ("Pigouvian tax") to encourage abatement

  e.g. $GHG\ tax = Emissions_{CO_{2,Eq}}\ €/ton_{CO_2}$

  ~80€/ton in 5/22

The weakness of either approach is that the damages can lead to increasingly catastrophic costs.

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Total operating costs

Therefore, the total costs are:

$$Total\ costs = \sum_i RM_i + \sum_j U_j + T + L + Supervision + Overhead + Maintenance + Rent + Plant\ overhead + SF + GHG\ tax$$

These costs are future costs. They will happen during the lifetime of the project.

They are offset by sales or savings (i.e. avoided costs). The yearly difference (hopefully positive) is the yearly cash flow.

The total yearly cash flow over the lifetime can be discounted to the present value to cancel the total capital cost, which will allow us to calculate the discounted rate of return.

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Time and money

The value of money changes depending on when it is available because any money spent now cannot be used to earn interest in a bank or investment. Money also loses value over time due to inflation. This can be accounted for by a rate of return (i).

Rate of return (compounded continuously)

$$F = P\, e^{it}$$

Time period

Future worth of *P*

Present cash flow

Conversely, the present worth of a future cash flow is:

Rate of return (compounded continuously)

$$P = F\, e^{-it}$$

Time period

Present worth of *F*

Future cash flow

This is for interest computed continuously… You are probably used to interest compounded once per year.

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Time and money

This is for interest computed continuously… You are probably used to interest compounded once per year.

Rate of return (discrete compounding)

Future worth of *P*

$$F = P\,(1 + i_d)^t$$

Time period (nb of years)

Present cash flow

If you compound *n* times per year: $F = P\left(1 + \frac{i_d}{n}\right)^{nt}$

Similarly, the present worth of a future cash flow is (for n=1):

Future cash flow

$$P = \frac{F}{(1 + i_d)^t}$$

Time period

Present worth of *F*

Rate of return (discrete compounding)

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Time and money

You can link continuous and discrete compounding:

$$i_c = \ln\left[1 + \frac{i_d}{n}\right]^n$$

E.g. for $n = 1$

$$F = P\,e^{i_c t} = P\,e^{t\ln[1+i_d]} = P\,e^{\ln[1+i_d]^t} = P[1 + i_d]^t$$

We can calculate the present value of all expenses for a process:

$$P_T = \sum_j F_j\,e^{-i_c t} \quad \text{or} \quad P_T = \sum_j \frac{F_j}{(1+i_d)^n}$$

Future cash flow at time t

We can then compute a levelized annual rate of expenditures A for a given continuous interest i_c, such that:

Lifetime of the technology

Levelized annual rate of expenditures

$$\int_0^T A\,e^{-i_c t}\,dt = P_T$$

Integrating and rearranging: $A = \frac{i_c}{(1 - e^{-i_c T})} P_T$

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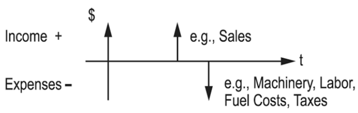
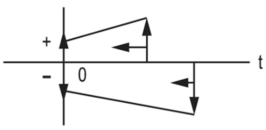
Minimum selling price or rate of return calculation

Here is the procedure to calculate the rate of return of a process or the minimum selling price of a product to make a given return:

1. Determine your cash flow (capital, operating costs, and revenue):





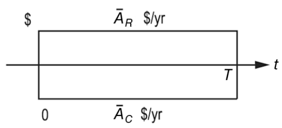
2. Bring all cash flows back to time zero and sum them up:

$$P_T = \sum_j F_j\,e^{-i_c t} \quad \text{or} \quad P_T = \sum_j \frac{F_j}{(1+i_d)^n}$$

3. Choose i_c/ i_d or alternatively the minimum selling price so that: $P_T = 0$

4. If of interest, redistribute all cash flows over the appropriate time horizon to calculate levelized annual costs and revenues:

$$A = \frac{i_c \sum_j F_j}{(1 - e^{-i_c T})}$$



→ They should be equal!

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