



Carbon Footprint Analysis at a Manufacturing Facility

AIChE Project Background Setup for CWRU Senior Capstone Internship

During Xellia Pharmaceuticals Spring 2020 Semester

AIChE Cleveland Section February 24, 2021 Meeting

Project Concept and Development:

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Presentation Overview:

- I. Dr. Bakshi's Sustainability Engineering Textbook Topics
 - A. Goal Definition and Scope
 - B. Inventory Analysis
 - C. Mathematical Framework
 - D. Footprint Assessment

II. CWRU Student Capstone Project at Xellia





Goal Definition and Scope

- I. Nature of Life Cycle Networks
 - A. Choose an environmentally friendlier transportation fuel that reduces reliance on fossil energy and CO2 emissions
 - B. Ethanol from corn fermentation is a good replacement for gasoline
 - C. Use ethanol as a fuel to reduce fossil fuel energy use and greenhouse gas emissions
- II. Steps in Assessing Life Cycle Networks
 - A. Goal Definition and Scope: For the Sustainability Assessment Study. Selecting the Functional Unit and defining the System Boundary
 - B. Inventory Analysis: Finding data for processes in the specified boundary
 - C. Impact Assessment: Utilizes the results of the Inventory Analysis to determine the impact of the selected system
 - D. Interpretation: Evaluate the pros and cons of the selected system over its life cycle. Used to identify opportunities for improvement.
- III. Goal Definition and Scope
 - A. For a sustainability assessment choose between options
 - B. Identify opportunities for improving a product or step
 - C. Functional Unit is used for a basis of comparison
- IV. Life Cycle Boundary
 - A. <u>Process Network</u>: most important process steps
 - B. <u>Input Output Network</u>: grouping of similar processes
 - C. <u>Hybrid Network</u>: Detailed network from A & B above



<u>Contributions to the Life Cycle Energy</u> used for a Car to obtain 1 Km of Mobility



Goal Definition and Scope



Calculation Example:

The goal in comparing ethanol with gasoline to choose between them from the perspective of mobility and what mixture of the two fuels that would provide the least CO2 and the best milage:

<u>GIVEN</u>:

- A. The fuel E10 is 10% ethanol and 90% gasoline
- B. The fuel E85 contains 85% ethanol and 15% gasoline
- C. E85 covers 20% less distance per volume of fuel than E10 due to a lower fuel value as well as the difference between the two engines using them
- D. Determine the functional unit for comparing the life cycles of these two fuels
- E. How much ethanol and gasoline will each vehicle use for the selected functional unit given the fuel economy of the E10 vehicle is 15 km/L

SOLUTION:

- A. The function of the E10 and E85 fuels is to provide mobility
- B. The Functional Unit may be the same distance traveled with either fuel, i.e. 100 km
- C. Determine the amounts of ethanol and gasoline needed for the selected Functional Unit: $\tilde{n} = 0.8 \times 15 \text{ km/L} = 12 \text{ km/L}$
- D. To drive 100 km with E10 requires: V(E10) = 100 km / 15 km/L = 6.67 L
- E. Since 10% of this is ethanol and 90% is gasoline, we get the volumes: V(E10, gas) = 6 L, and V(E10, EtOH) = 0.67 L
- F. Similarly to drive 100 km with E85 we get: V(E85) = 100 km / 12 km/L = 8.33 L
- G. Therefore: V(E85, gas) = 1.25 L and V(E85, EtOH) = 7.08 L

Life Cycle Boundary

- A. Process Network Model: Dark Circles Most Important Process steps (PI – P4) for a Corn to Ethanol Process
- **B.** Input Output Network Model: Similar Process Steps lumped together into Sectors (S1 S5) for a Corn to Ethanol Process
- **C. Hybrid Network Model**: Combine A & B above with details from both A & B networks







B. Input – Output Network

C. Hybrid Network



Goal Definition and Scope



- D. Selected Processes in Corn to Ethanol Life Cycle Network Model
- E. Selected Economic Sectors in the Input Output Corn to Ethanol Life Cycle Network Model
- F. Hybrid Network model combining the Process Network and the Input Output Network Models
- G. Note that the Economic Sectors are tagged with the North American Industrial Classification System (NAICS)



D. Process Network Selected Processes

E. Input – Output Network with Selected Economic Sectors F. Hybrid Network Combining Selected Processes & Economic Sectors

Inventory Analysis

I. Sources of Data

- A. Calculations with Life Cycle Network models require data about the selected activities and their flows: Life Cycle Inventory (LCI)
- B. Over the past years the LCIs for a large variety of systems have been compiled and have become available as free and commercial databases
 - i. National Renewable Energy Laboratory. US Life cycle inventory database <u>www.lcacommons.gov/nrel/search</u>, accessed November 3, 2014
 - Argonne National Laboratory. The greenhouse gases, regulated emissions, and energy use in transportation (GREET) model <u>http://greet.es.anl.gov</u>, accessed January 31, 2012
 - iii. Swiss Center for Life Cycle Inventories. Ecoinvent life cycle inventory database <u>www.ecoinvent.ch</u>, accessed January 18, 2013
 - iv. Environmental Protection Agency. National emissions inventory, Toxics release inventory www.epa.gov/ttn/chief/trends, www.epa.gov/triexplorer, accessed August 22, 2015
 - v. Food and Agriculture Organization. FAOSTAT <u>http://faostat3.fao.org</u> , accessed July 8, 2017

II. Calculations

- A. With LCI data for multiple processes we can calculate various quantities for the entire life cycle network formed by connecting the process modules
- B. The data in each process module are usually normalized to a unit output of the primary product
- C. It should be easy to determine the scaling factors for each module in order to connect them to obtain results for the selected functional unit
- III. Uncertainty: Parametric (inherent variability in measured data), Scenario (modeler value judgement), Model (simplified)



Inventory Analysis

Calculation Example (converting crude oil into electrical power):

<u>GIVEN:</u>

- A. Module PI for fuel production has an input of 50 L of crude oil to produce 20 L of fuel
- B. It emits 2 kg SO2 and 10 kg CO2
- C. Module P2 for electricity generation produces 10 kWh of electricity from 2 L fuel
- D. It emits 0.1 kg SO2 and 1 kg CO2
- E. For a network constructed by connecting these modules, determine the life cycle consumption of crude oil and the emissions of SO2 and CO2 generating 1,000 kWh elec.

<u>SOLUTION</u>:

- A. To generate 1,000 kWh of electricity, P2 needs to be scaled by 1000/10 = 100
- B. This scaled up module will need 200 L of fuel
- C. To supply this fuel PI needs to be scaled by 200/20 = 10
- D. The resulting Life Cycle Network is shown in the following diagram
- E. In this diagram the total consumption of crude oil is ${\bf 500}~{\rm L}$
- F. The emissions of SO2 = 30 kg and CO2 = 200 kg







Inventory Analysis



Calculation Example (environmental impact generating electrical power):

<u>GIVEN</u>:

- A. Use the Input Output Data in the **Table I** to the right
- B. Determine the Life Cycle emissions and resource use in the generation of 500 kWh of electricity in the USA
- C. The producer price of electricity is 5 cents/kWh $\,$

SOLUTION:

- A. The producer price of electricity is 500 kWh x 0.05 = 25
- B. This is the final demand of electricity
- C. Multiplying the coefficients for the electricity sector in **Table I** to the right by this price gives the Life Cycle Flows of:
 - i. CO2 to air = \$25 x 6.27E00 = <u>156.75 kg</u>
 - ii. Cropland = 25×6 ; $24E-03 = 0.156 \text{ m}^2 \text{ yr}$
 - iii. Benzene to air = $25 \times 1.62E-05 = 4.05 \times 10^{-4} \text{ kg}$
 - iv. Glyphosate to water = $25 \times 1.02E-08 = 2.55 \times 10^{-7}$
 - v. Groundwater = \$25 x 6.35E-03 = <u>0.16 m^3</u>

Table I:Typical Life Cycle Inventory data from Input-Output Models Reference: Y.Yang, W.W. Ingwersen, T.R. Hawkins, M. Srocka, and D.E. Meyer USEEIO: a new and transparent United States environmentally extended input-output model. *Journal of Cleaner Production*, 158:308-318, 2017

	FLOW	Wheat, Corn,	Electricity	Gasoline etc.	Couriers	Management	: Vehicle
		etc.				Consulting	Repair
	(NAICS)>	(b0)	(221100)	(324110)	(492000)	(541610)	(811100)
	CO2 to ai (kg / \$)	r 1.28E+00	6.27E+00	5.03E-01	I.82E01	9.97E-02	1.53E-01
I	Cropland (m^2Yr / \$)	1.19E+01	6.24E-03	6.38E-03	6.63E-03	5.77E-03	5.35E-03
	Benzene t Air (kg / \$)	o 2.20E-05	I.62E-05	6.14E-05	8.65E-06	I.75E-06	2.09E-06
	Glyphosat To water (kg / \$)	æ 2.95E-05	I.02E-08	I.17E-08	9.86E-09	I.04E-08	8.05E-09
	Groundwa (m^3 / \$)	ater 3.71E-01	6.35E-03	2.82E-03	I.03E-03	7.12E-04	9.98E-04

Mathematical Framework



- A. Process Network Analysis
 - i. Mathematical Framework
 - a. Previous calculation examples are basic models and easily scaled
 - b. For more complicated models a more rigorous approach is needed
 - c. Life Cycle modules contain two types of flows: economic and environmental
 - i. Economic Flows generated by human activity are used in other economic activities Such flows are valuable to society and are not discarded directly into the environment This would be the Fuel and Electrical power flows (the Final Demand) from our example
 - **ii. Environmental Flows** are inputs from nature and emissions into it These would be the Crude Oil flow from the environment and the SO2 and CO2 flow into it

ii. Allocation Methods

- a. Partitioning: requires splitting a process with multiple products into multiple processes each with a single product
- b. Displacement: required data about a conventional process that produces each byproduct
- c. No Allocation: in the absence of allocation, all allocation weights are taken as equal to 1
- B. Input-Output Analysis: overcome shortcoming of process network analysis, has larger analysis boundary with less accuracy
 - i. Mathematical Framework: consists of a collection of nodes of various sectors with monetary flows between sectors
 - ii. Environmentally Extended Input-Output Models: for assessing environmental impacts from monetary flows in sectors
- C. Hybrid Models: combines the features of the Process Network and the Input-Output Network

Mathematical Framework

Theory (Matrix Notation):

- A. Economic Flows Fuel and Electricity have a final demand
- B. Let f1 and f2 represent the final demand of these two flows in our Crude Oil to Electrical Power Example
- C. The final demand for fuel is 0, and the final demand for electrical power is 1,000 kWh
- D. Let s1 and s2 be our scaling factors for these two modules
- E. We can write two equations based on the conservation of each economic flow:

i. Eq. 1, 20s1 - 2s2 = f1 ii. Eq. 2, 10s1 = f2

- F. Eq. I is for fuel and represents fuel produced is 20s1, and fuel used is 2s2
- G. Eq. 2 is for electricity and represents electricity produced is 10s2

H. In matrix notation as:

 $\begin{vmatrix} 20 & -2 \\ 0 & 10 \end{vmatrix} \begin{vmatrix} s1 \\ s2 \end{vmatrix} = \begin{vmatrix} f1 \\ f2 \end{vmatrix}$ or, more generally, as **As = f** Where **A** is the **Technology Matrix**

I. For the Environmental flows we have similar balance equations:

i.Eq. 3, rCrude = -50s I $|-50 \ 0 |$ |rCrude |ii.Eq. 4, rSO2 = 2s I + 0.1s2 $2 \ 0.1 |$ |sI| = |rSO2 |iii.Eq. 5, rCO2 = 10s I + s2or in matrix notation: $|10 \ 1 |$ |s2| ||rCrude |rCO2with **Bs = r**

Where **B** is the **Intervention Matrix**

- J. Where ri is the total Environmental Flow of the i th component. With negative signs are inputs and positive signs as outputs
- K. Where r is the vector of **Resource Consumption and Emissions**. Where: r = BA^(-I)f



Mathematical Framework



Calculation Example (solving previous example with matrix notation):

GIVEN:

- A. Consider the fuel and electricity modules in our previous example
- B. Calculate the Life Cycle Flows of crude oil, sulfur dioxide, and carbon dioxide in the production of 1,000 kWh of electricity

SOLUTION:

- A. The Final Demand is specified as fI = 0 and f2 = 1000 kWh
- B. Solving Eq. I and Eq. 2 simultaneously, we find the scaling factors sI = I0 and s2 = I00
- C. Substituting the scaling factors in Eq. 3, Eq. 4, and Eq. 5 we get rCrude = -500L, rSO2 = 30 kg, and rCO2 = 200 kg
- D. Using matrices, define f = 0
 - The resource consumption and emissions can then be expressed as $r = \begin{bmatrix} -500 \\ 30 \end{bmatrix}$
- Ε.
- Where the Crude Oil = 500 L, SO2 = 30 kg, and CO2 = 200 kg as found in the previous calculation example F.

Footprint Assessment

- A. Carbon Footprint
 - i. Global Warming Potential (GWP) relative to CO2
 - a. If we consider a 100 year time period
 - b. Methane is 25 times more potent than CO2
 - c. Nitrous Oxide is 298 times more potent than CO2
 - d. Their potency changes with time each gas lasts in the atmosphere
 - e. In 2016 in terms of CO2 equivalents the atmosphere contained 489 ppm CO2 eq, an increase of 40% since 1990 (or over 26 years)
 - ii. Greenhouse Gas (GHG) Emissions
 - a. Data about GHG emissions from various human activities are compiled in public and private databases
 - b. The US Environmental Protection Agency compiles data about GHG flows in the USA and the world <u>www.epa.gov/ghgemissions/inventory-us-greenhouse-gas-emissions-and-sinks-1990*2016</u>
 - c. In 2016 total USA emissions were ~6.5 billion tons of CO2 eq. with sequestration at ~1 billion tons CO2
 - d. An overshoot of ~5.5 billion tons of CO2 eq. in 2016 above nature's capacity to sequester CO2 in USA
 - e. This CO2 will be sequestered by ecosystems in other parts of the globe or accumulate in the atmosphere
 - f. The boundary of Carbon Footprint calculations is classified as Scope 1, 2, or 3
 - i. Scope I is a narrow boundary for direct GHG emissions from selected processes
 - ii. Scope 2 includes GHG emissions in generating electricity and those caused by heating the processes
 - iii. Scope 3 is the full Life Cycle of GHG emissions



Footprint Assessment

B. Water Footprint

- i. Direct and Indirect dependence of products, processes and other systems on water
- ii. Important for water intensive activities in water stressed regions of the world
- iii. Water Footprint relies on the concept of Virtual Water (water used to make a product or service)
 - a. Virtual Water use in thermal power is mainly due to evaporative losses and leaks
 - b. Virtual Water use in a beverage is the water contained in it
 - c. Water withdrawn and returned to the environment in a form it can be used directly is not Virtual Water
- iv. The Water Footprint is the sum of direct and Indirect virtual water flows
 - a. Water Footprint of thermal electricity includes the water used in the steps of its Life Cycle such as mining and cleaning coal, producing solvents used for scrubbing the flue gas, manufacturing of equipment, etc.
 - b. For a geographic region or nation, its Water Footprint accounts for the virtual water in imports and exports along with the water use in the region
- C. Sources of water and changes in quality based on following categories of water:
 - i. Blue Water: Includes fresh water available at the surface in rivers, lakes, canals, and groundwater
 - ii. Green Water: Precipitation that falls on land and does not runoff or recharge the aquifer
 - iii. Gray Water: Focuses on the quality of water needed to dilute pollutants to acceptable levels Gray Water quality is from a material balance calculation with information about the current and desired concentration of contaminants in the water. Where P = pollutant loading (mass/time),

Cmax = max contaminant loading (mass/volume), and

Cnat = natural concentration of this contaminant in the environment

Then the Gray Water Footprint for this flow may be calculated as: Wgray = P / (Cmax - Cnat)

Footprint Assessment

Calculation Example (determine the Global Warming Potential, GWP, from a Life Cycle Inventory of emissions with Table 2):

<u>GIVEN</u>:

- A. Table 2 to the right
- B. Life Cycle Inventory emissions
- C. Determine the GWP using a 100 year time horizon

<u>SOLUTION</u>:

- A. Using **Table 2**, the GWP of these emissions is $GWP = (20 \times 1) + (0.001 \times 4750) + (0.5 \times 298)$ GWP = 173.8 kg CO2 eq
- B. Note that NO2 does not contribute to global warming and is excluded from this calculation

Table 2: Global Warming Potential relative to CO2

P. Forster, V. Ramaswamy, P. Artaxo, et al. Changes in atmospheric constituents and in radiative forcing. Ln S. Solomon, D. Qin, M. Manning, et al., editors, *Climate Change 2007: The Physical Science Basis. Contribution of Working Group 1* to the Fourth Assessment Report of the Intergovernmental Panel on Climate *Change.* Cambridge University Press, 2007

Common Name	Chemical	GWP for given time horizon
	Formula	100 Year
Carbon Dioxide	CO2	I
Methane	CH4	25
Nitrous Oxide	N2O	298
CFC-11	CCI3F	4750
Carbon Tetrachlori	de CCl4	1400
HCFC-22	CHCIF2	1810
HFC-134a	CH2FCF	-3 1430
Sulfur Hexafluoride	e SF6	22,800
Methyl Chloride	CH3CI	13



CWRU Student Capstone Project

Kickoff Meeting with four ChE Senior Students Non-Disclosure Agreement review and sign-off Xellia Plant Tour

Scope of Work review and sign-off

Project Schedule and Deliverables review and sign-off







Carbon Footprint Analysis at Xellia

Sanjana Kamath, Nathan Ewell, Katie Francissen, Andy Swyers CWRU Capstone Project

CWRU Capstone Project Concept and Development by: Joseph Yurko, PE AIChE Fellow

Meet the Team





Nathan Ewell



Katie Francissen

Andy Swyers



Sanjana Kamath

CWRUcible, Inc.



The Crippling Effects of Climate Change



Economical Environmentalism



ESG is Environmental, Social Governance

Of 200 studies analyzed by Arabesque and University of Oxford...



90% conclude that good ESG standards lower the cost of capital



88% show that good ESG practices result in better operational performance



80% show that stock price performance is positively correlated with good sustainability practices

Project Objective and Scope

- Carbon footprint analysis of building 22
 - Convert process loads into CO₂ equivalents
 - Assess overall environmental impact
 - Pinpoint areas of improvement



Methods: Carbon Footprint Analysis





Chemicals in the atmosphere absorb solar radiation, warming the earth

Chemical	20 year GWP	100 year GWP	500 year GWP
Carbon Dioxide	1	1	1
Methane	72	25	7.6
Nitrous Oxide	289	298	153

Global warming potential (GWP) can be defined for chemicals relative to CO₂

Activity	CO ₂ Factor (kg/unit)	CH₄ Factor (kg/unit)	N ₂ O Factor (kg/unit)	Unit
Natural Gas Combustion	1.922	0.036	0.004	m ³
Electricity Usage (midwest)	564	0.050	0.0086	MWh

Methods: Projecting Utility Usage





Building 22 Carbon Footprint

- Overall carbon footprint = 31,000 mt CO₂ eq.*
- Broken down into two major categories
- \rightarrow Natural gas: 17,000 mt CO₂ eq.
- \rightarrow Electricity: 14,000 mt CO₂ eq.

*20 year global warming potential

Average American Car has a carbon footprint of 4.6 mt CO₂ per year (Source: EPA)







Annual Usage Breakdown: Natural Gas

- Almost half of NG consumption from boilers
- Other major contributors*
 - Water/steam heaters
 - Kitchen equipment
 - HVAC units/space heating

*Estimates for non-boiler components were based on capacity values





Long Term Impacts

- Small decrease in carbon footprint as gases decay
- Electricity use has more persisting impact



Water Footprint

- Water usage was broken down in terms of:
 - Contribution due to boilers and other equipment
 - Batches produced per week

		Batches/week	c .
	1	1.5	2
Water footprint (gal/batch)	780,000	520,000	390,000



Annual Electricity Usage Breakdown: Lyophilizer



- Analyzed electricity consumption of different components of lyo process
- 440 mt CO2 eq. emitted per year
- Heating element is primary contributor



Recommendations: High Efficiency Boiler*



Environmental BenefitsEconomic Benefits• 13.7% reduction in natural gas
usage due to boilers
→ 6% reduction in carbon
footprint due to natural gas
→ 3% reduction in overall carbon• Reduced natural gas usage
→ Annual savings of \$13,000

*Calculations based on boiler with 95% efficiency Current boiler has efficiency of 82%

footprint

Recommendations: Continual Updating of Spreadsheet



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9		Scaling Factor (Water)	Calculation of utility scaling factor based on projected water use and historical use					
-		Scamp ractor (water)	Estimated water footprint per batch,					
10		Water Use and Footprint	estimated water footprint breakdown		Tab for each com	nonent of		
11		Steam Use	Estimated steam use		Tab for each com	iponent of		
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16		Lyophilizer Carbon Footprint	lyophilization process					
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Other Recommendations



Recommendation	Outcome
Manipulate control of compressor	 Reduced use of backup compressor Reduced electricity waste
Renewable sources of electricity	 Reduce long-term carbon footprint
Breakdown of electricity use	 Identify areas of improvement







Estimated footprint of 31,000 mt/year CO2 eq.



Simple actions can reduce environmental impact and result in cost savings



Improve upon projections using additional data



Apply methods to other processes on site

Acknowledgments

- The Xellia team: Kruttika Patel, Frank Medina, and Jeffrey Bores
- CWRU advisors: Prof. Uziel Landau and Prof. Daniel Lacks
- Others: Joe Yurko AIChE Consultant





Environmental Footprint Assessment:

Xellia Pharmaceuticals



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	20	20 Capstone Inte	ernship Cert	ificate
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		The Cleveland, Ohio Ma	EUTICALS anufacturing Facility	of
	Xe	ellia Pharmaceu	ticals USA,	INC.
		Is pleased to recog	nize and present	
Fer	the 2020 Co	Nathan		sible Team as formin
For	Sustaina	ble Engineering Ca	bon Footprint	LCA Project
		supervised by Jo in conjund	seph Yurko, P.E.	
	AIChE	and the Department of Chemic	cal and Biomolecular E	Engineering at
	Case W	estern Reserve Univ	ersity School of	Engineering
		this 18th day of	April, 2020	
		Datal Disc Delayda D E	Branda Shular	Barton Farmer, P.E.





- B. R. Bakshi, *Sustainable engineering: principles and practice*. Cambridge, United Kingdom: Cambridge University Press, 2019.
- Emissions & Generation Resource Integrated Database, EPA, 2018