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Integrated Open Source Life Cycle Assessment of Electricity Generation Technologies

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Integrated Open Source Life Cycle Assessment of Electricity Generation Technologies

by

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Thesis

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Dedication

I would like to dedicate this thesis to my beloved wife and to the memory of my beloved mother.

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I would like to express my sincere gratitude to Dr. Carey King for his continuous guidance over the course of this research. Dr. King’s teaching, patience, understanding of concepts, knowledge and help has enabled me to complete this thesis.

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Abstract

Integrated Open Source Life Cycle Assessment of Electricity Generation Technologies

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Energy return ratios help us to understand the influence of energy on the growth, structure and organization of societies. Energy return ratios also help assess the likelihood of new technologies in terms of sustainability and their influence on economic growth. Net energy analysis is part of Life Cycle Assessment and calculates Energy return ratios of energy systems. In this thesis, we have created LCA models for multiple electricity technologies using data from (Hertwich et al. 2015). The LCA models are integrated to create a system-scale LCA model. Energy return ratios for all the models are calculated using the LCA models representing electricity generation technologies and for the integrated LCA model. We have developed a scalable, object oriented, open source methodology that allows for expansion of the integrated system-scale LCA model and also enable creation and analysis of any other LCA model.

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Introduction

Life Cycle Assessment (LCA) is an effective tool for analyzing future electricity generation scenarios. Metrics like resource usage over the lifetime of the system or the product is computed using LCA. LCA has an added advantage over economic analyses because the latter do not include some impacts like Greenhouse gas emissions, land usage, ecotoxicity and other environmental impacts. Net energy analysis is performed using LCA and is used to calculate energy return ratios (Brandt et al. 2011, Raugei et al. 2012, Brandt et al. 2013, King 2014, Arvesen and Hertwich 2015). The study presented in (Hertwich et al. 2015) calculates material flows and non-renewable energy demand by integrating twenty-one electricity generation technologies. However, the study presented in (Hertwich et al. 2015) does not compute energy return ratios. In this thesis, twenty-one LCA models are developed using data from (Hertwich et al. 2015) representing twenty-one electricity generation technologies. These models are then integrated to develop a single LCA model. A common methodology is developed that enables calculation of energy return ratios for all the LCA models. This thesis also presents an open source methodology that enables expansion and improvement of the integrated LCA model.

BACKGROUND OF LIFE CYCLE ASSESSMENT AND ENERGY RETURN RATIOS

Life Cycle Assessment (LCA) is a widely used methodology used to measure resource use (materials and energy) and environmental impacts over the lifetime of a system (Sanden and Arvesen 2014) or a product, where a product can mean goods or services (Finnveden et al. 2009). LCA has been employed in various sectors of the society and the economy like policy and decision making at various levels from government to the corporations (Hellweg and Canals 2014), analysis of new and existing energy sources (Aresta et al. 2005, Pehnt 2006, Martinez et al. 2009) and analysis of new and existing electricity supply technologies (Mann and Spath 2001, Odeh and Cockerill 2009, Espinosa et al. 2011, Raugei et al. 2012). LCA is used extensively in determining the environmental impact (e.g., emissions, land use, ecotoxicity etc.) over the lifetime of various systems or products (Reap et al. 2008, Hellweg and Canals 2014, Hertwich et al. 2015). Apart from measuring resource use and environmental impact, LCA is used to calculate energy usage and energy return ratios. Cumulative Energy Demand (CED) is an energy metric of that is generally computed using LCA methodologies and represents the total direct and indirect energy used over the life time of the energy system (Hujibregts et al. 2010). Energy return ratios are calculated using LCA models either using CED (Sanden and Arvesen 2014) or using inventory data that makes up the LCA model (Raugei et al. 2012, Brandt et al. 2013). Energy Return Ratios (ERRs) refer to a set of energy metrics that are defined to quantify the energy input and output relationship obtained from an energy generation systems and technologies. ERRs are one type of metric that can be calculated from life cycle analysis (LCA) that is often more focused on environmental analysis of products and processes that can include energy systems, fuels, and electricity generation technologies (Sanden and Arvesen 2014). The term ERR is a generic term for more specific calculations of energy output divided by energy inputs required to make that output. In short, energy analysis and the calculation of ERRs can be considered a subset of LCA.

In the past and current literature, Energy Return Ratios have been interpreted for importance within various different contexts and boundary considerations: societal (Hall et al. 2009), anthropology-based societal organizational (Tainter et al. 2003), economical (King 2014) and social (Lambert et al. 2014). More specifically in the context of energy systems, ERRs have been used to compare different fuel sources (Cleveland 2005, Hammerschlag 2006, Gately 2007, Gagnon 2009, Hall et al. 2009, Dale et al. 2011), electricity producing technologies (Heller et al. 2004, Kubiszewski 2010, Raugei et al. 2012, Weissbach et al. 2013), and system-scale energy efficiencies of a combination of technologies (Brandt et al. 2013, King et al., 2015).

Tainter et al. (2003) defines energy gain as the difference between of energy extracted and the energy invested to gain that energy. Energy, in general or energy gain, in particular, "influences the structure and organization of living systems" (Tainter et al. 2003). Measuring energy return ratios at the societal level, helps in understanding the influence of energy on society's growth, structure and organization (Tainter et al. 2003, King et al. 2015). Calculating energy return ratios of energy technologies helps in understanding how future technologies can influence society's economic growth, structure and organization.

In the most general form, the energy return ratios are defined as the ratio of the energy output to the ratio of energy used to deliver the energy to the society (King et al. 2015). There are different variations of energy return ratios and the difference between these ratios stem from the differences in the way the numerators and the denominators that make up the ERRs are defined. Some of the different types of ERRs used in the past and current literature are EROI (Energy Returned On Investment) (Hall et al. 2009), Net Energy Ratio, Gross Energy Ratio, Net External Energy Ratio and Gross External Energy Ratio (Brandt et al. 2011, Brandt et al. 2013, King 2014, King et al. 2015). The definitions of these ratios are provided in future sections of the thesis.

EROI is a widely used and an important metric representing energy return ratios and has various applications. Societal EROI, as defined by (Hall et al. 2009), can be used to analyze the sustenance of a society. Studies have shown that the increase in EROI correlates to improved social and quality of life indicators like GDP per capita, human development index, literacy rate and gender inequality index (Lambert et al. 2014). From the perspective of energy generation systems, economic and energetic EROI will help analyze if the energy system is a net source or a sink of useful energy to the society (Arvesen and Hertwich 2015). The energy ratios in general and EROI in particular can "also help illuminate two important aspects of an energy system: the quality of the energy resource being extracted, and the ingenuity with which humans extract that energy" (Brandt et al. 2011).

Often EROI is used too broadly because of the variations in the mathematical definitions of the same (King et al. 2015). Also, the usefulness of the EROI depends on the definition of the numerator and denominator that make up the energy ratio (Brandt et al. 2011). Net Energy Ratio (NER) and Net External Energy Ratio (NEER) provide more standardized definitions of energy return ratios by specifying what should be in the numerator and what should be in the denominator. Net Energy Ratio is the ratio of energy output to the total energy consumed (Brandt et al. 2011, King 2014). Net External Energy Ratio is defined as the ratio of energy output to the total energy consumed excluding any energy converted to waste heat as direct energy from any primary energy source feedstock converted to an energy carrier output (Brandt et al. 2011, King 2014). EROI refers to the definition of NEER (specified mathematically later). NER and NEER serve the same role that EROI plays in helping quantify various benefits from an energy system. In addition, NER and NEER also help in identification and differentiation of energy systems that require less energy from the society from those that require more (Brandt et al. 2011). Systems that use less external energy from the society have higher NEER values than other systems indicating that they are self-fueling systems (Brandt et al. 2011, King 2014).

Gross Energy Ratios viz. Gross Energy Ratio (GER) and Gross External Energy Ratio (GEER) are gross equivalents of the NER and NEER. GER is defined as the ratio of gross energy output to the total energy consumed. Gross energy output of a system is the sum of energy output from the system and the total energy consumed by the system. Gross energy is also the total primary energy extracted from the Earth required to power the modeled processes. GEER is defined as the ratio of the gross energy output to the total energy consumed excluding the energy from the primary energy source feedstock (Brandt et al. 2011, King 2014).

There are several papers describing methods for calculating energy return ratios (Cleveland 2005, Heller et al. 2004, Hammerschlag 2006, Gately 2007, Gagnon 2009, Hall et al. 2009, Dale et al. 2011, Kubiszewski 2010, Brandt et al. 2011, Raugei et al. 2012, Brandt et al. 2013, Weissbach et al. 2013, King 2014, Arvesen and Hertwich 2015). However, majority of the available literature calculate energy return ratios for specific energy systems (Cleveland 2005, Heller et al. 2004, Hammerschlag 2006, Gately 2007, Gagnon 2009, Dale et al. 2011, Kubiszewski 2010, Raugei et al. 2012, Weissbach et al. 2013). As a result, methodologies available for different energy sources are different. (Brandt et al. 2011) propose a generic methodology to compute energy return ratios for any energy system. We discuss this methodology further because it provides two advantages – first, the possibility of using the same framework consistently for multiple electricity generation technologies to compute energy return ratios and perform comparison of these electricity generation technologies and second, the possibility of computation of all indirect impacts that are associated with the inputs to the system.

SCOPE OF THIS THESIS

The main scope of our research is to compute energy return ratios for individual electricity producing technologies as well as at the system-scale by considering current and future electricity supply mix scenarios.

The majority of the studies in the current literature have focused on computing energy return ratios for specific energy systems by analyzing them individually (Cleveland 2005, Heller et al. 2004, Hammerschlag 2006, Gately 2007, Gagnon 2009, Dale et al. 2011, Kubiszewski 2010, Raugei et al. 2012, Weissbach et al. 2013). As a result, methodologies developed for different energy sources vary significantly. While energy return ratios computed using individual models that have consistent system boundary definitions and comprehensively account for all energy inputs (within the boundary) can be used to compare multiple electricity generation technologies, it is desirable to have a harmonized method of computing energy return ratios for multiple electricity generation technologies. (Hertwich et al. 2015) follow a consistent and comprehensive methodology to compute material flows and cumulative energy demand for multiple electricity generation technologies, but have not performed computations of energy return ratios. (Arvesen and Hertwich 2015) understand and recognize that the study in (Hertwich et al. 2015) does not perform energy return ratio computation. However, (Arvesen and Hertwich 2015) have not performed computation of energy return ratios. Our research seeks to use the data from (Hertwich et al. 2015) to perform energy return ratio computation for various electricity generation technologies.

(Hertwich et al. 2015) compute CED for various electricity generation technologies. When these CED values are used to compute NEER using the (Arveson and Hertwich 2015) method, some of the results are inconsistent with the expected range of calculated values (e.g the NEER for coal power plants for some regions is less than 0) (This calculation NER from CED is described in the Design chapter). This brings into question the validity of CED results presented by (Hertwich et al. 2015). Therefore, our research seeks to apply the (Brandt et al. 2013) framework to inventory data from (Hertwich et al. 2015) to compute energy return ratios at subsystem-scale and system-scale instead of using the (Arveson and Hertwich 2015) method applied to CED from (Hertwich et al. 2015).

While, the main focus of the research is on energy return ratios, our research also seeks to compare the material and emissions flows to the results reported by (Hertwich et al. 2015) in order to understand how far off our models are from the (Hertwich et al. 2015). The reason our calculations should produce different, mainly lower quantities of energy and material needs, as compared to (Hertwich et al. 2015) is that our analysis is missing much of the input data used by (Hertwich et al. 2015). Many of the (Hertwich et al. 2015) inputs were obtained from the proprietary Ecoinvent database, and thus are not provided in the supplemental information of (Hertwich et al. 2015).

Lastly, our research seeks to make all the subsystem-scale and system-scale LCA models and methodology open source for the net energy community to add data and build upon the models in order to refine energy return ratio computations.

GOALS AND OBJECTIVES

Integrated LCA model

The goal of this research is to develop an integrated open source LCA model encompassing multiple electricity generation technologies using data from (Hertwich et al. 2015) to enable calculation of material and energy flows.

Energy Return Ratios

The goal of this research is to develop a harmonized methodology to compute energy return ratios using subsystem-scale and system-scale LCA models for different electricity generation technologies.

Open source LCA methodology

The goal of this research is to provide an open source LCA methodology that will enable expansion and improvement of the unified system-scale LCA model by adding data and processes. The open source methodology is also required to enable creation of any LCA models and performing LCA assessment and ERR computation. Some of the important characteristics of an open source LCA methodology are

1. Use of main-stream tools like Microsoft Excel to develop subsystem-scale or system-scale LCA models.
2. Use of main-stream tools like Matlab to develop programs that implement functionality pertaining system-scale model creation, LCA and energy ratio analyses.
3. A simple way of specifying processes of a LCA model, the required matrices for LCA and energy ratio analyses.
4. A simple way of creating new LCA models or adding processes and data to existing LCA models.
5. A scalable way of creating and analyzing system-scale models that contains large number of processes.

ORGANIZATION OF THE THESIS

The rest of this thesis is organized into four chapters – Design, Implementation, Results, Discussion and Appendix A . The methodology designed for LCA assessment and energy return ratios computations are described in the Design chapter. The Implementation chapter includes a description of the source and organization of data, list of software tools used, description of source code and programs. The Results chapter presents a description of the unified, system-scale LCA model that encompasses twenty-one electricity generation technologies. Additionally, it also includes the results of LCA assessment and energy return ratio computations for subsystem-scale and system-scale LCA models. Lastly, the Discussion chapter presents an analysis of the results and goals for future work. The object oriented methodology and algorithms designed to create the system-scale LCA models is described in Appendix A.

Design

The system or subsystem under consideration is modeled as a LCA system comprising of a set of interdependent processes. Each process is modeled as a single column, and corresponding row, in a matrix of all processes. Each process describes the necessary inputs for producing some output such as a material, energy carrier, or economic service. Environmental flows are also associate with each process and organized into a different matrix. Life Cycle Inventory analysis (LCI) is the first part of the overall LCA methodology that involves compilation of the inputs and outputs of the pathways (Suh 2005). The process of LCI will primarily result in two matrices that make up the LCA model. The technology matrix, also referred to as the **A** matrix, represents processes for material and energy flows of the LCA system (Heijungs and Suh 2002, Brandt et al. 2013). The intervention matrix, also referred to as the **B** matrix, represents the environmental flows (like pollutants) of the LCA system (Heijungs and Suh 2002, Brandt et al. 2013). In order to complete the model and enable net and gross energy analysis, the demand vector, also referred to as the **f** vector, is defined and it represents the desired material or energy output from the LCA system (Heijungs and Suh 2002, Brandt et al. 2013). The matrix based methodology calculates all indirect impacts that are associated with the inputs to the system and all environmental flows (into the economy from the environment and from the economy into the environment) due to the provision of final demand.

Object oriented methodology is used to convert the data from (Hertwich et al. 2015) to create subsystem-scale and system-scale LCA models. This methodology, including all the algorithms we have developed, is described in Appendix A.

After the system-scale LCA models were created, two processes were added – "General primary energy" and "Electricity Supply from Grid". "General primary energy" process contains energy inputs required for material production and extraction that are not provided in the original data but are provided by the supplementary information in (Hertwich et al. 2015). More specifically, this process captures the non-electricity based energy required to extract metals like Aluminum, Copper, Nickel, Pig iron and manufacture materials like glass and metallurgical grade silicon. If the process has an electricity based energy input, it is added to the "Electricity supply from Grid" process. The "Electricity supply from Grid" process is used link the electricity input for some processes in the LCA model to the outputs produced by the model. For example, in the system-scale LCA model, grid electricity is used as an input to the process that represents the installation of the cables required for a roof-mounted PV poly-Si electricity generation system. Using the "Electricity supply from Grid", the input electricity to the process the represents installation of cables is linked to the output of the system viz. electricity from a combination of technologies like Coal, Natural gas, Hydro etc. For the "Electricity Supply from Grid", we have assumed that 35% of electricity comes from Gas, 40% from Coal (IGCC without CCS), 15% Hydro and 10% from PV Poly-Si (Roof). Using these two processes, and the Waste Heat vector (described later), all direct and indirect energy required by the LCA model is accounted for.

LCA ASSESSMENT

Matrix based LCA assessment described in (Heijungs and Suh 2002) (Brandt et al. 2013) is used to perform LCA assessment on the subsystem-scale and system-scale LCA models developed using the methodology above. Equations (1) and (2) are used to perform the LCA assessment (Heijungs and Suh 2002) (Brandt et al. 2013)

$$\mathbf{s} = \mathbf{A}^{-1}.\mathbf{f} \tag{1}$$

$$\mathbf{g} = \mathbf{B}.\mathbf{s} \tag{2}$$

The **f** vector represents the demand for the required outputs. $\mathbf{A}^{-1}$ is the inverse of the **A** matrix. **s** vector is the called the scaling vector. The scaling factor of each of the unit processes required to produce f in the **s** vector. The **g** vector is called inventory vector and represents the emissions that are a result of meeting the demand of the outputs in the **f** vector.

ENERGY RETURN RATIOS

Energy return ratios described in (Brandt et al. 2013, King 2014) are calculated using LCA system-scale and subsystem-scale models. The energy ratios are categorized into two types depending on the type of output energy computed – Net and Gross. The energy ratios are further categorized into two types depending on whether feedstock is included as an input. Table 1 shows the four types of energy ratios. Factors like Total Energy Demand, Total Waste Energy and Total Feedstock Energy are calculated in order to obtain the energy ratios.

	Feedstock included as input	Feedstock not included as input
Gross	Gross Energy Ratio (GER)	Gross External Energy Ratio (GEER)
Net	Net Energy Ratio (NER)	Net External Energy Ratio (NEER)

Table 1: Types of Energy Return Ratios (King 2014)

Energy ratios are calculated using two methods. Method 1 is developed based on the bottom-up framework proposed by (Brandt et al. 2013). Method 2 uses the methodology proposed in (Arvesen and Hertwich 2015) using CED

Method 1: Based on the Bottom-up framework (Brandt et al. 2013)

Total Energy Output (TEO)

Energy Output, as well as the required outputs of products from non-energy processes, are represented in the **f** vector. However depending on the way the processes are defined, the **f** vector may possibly include energy outputs that are not represented in units of energy (like MJ). Typically, outputs like electricity are represented in units of kWh. In order to convert units of electricity to other energy units (like MJ), a one-dimensional Energy Conversion Factor (ECF) vector is defined. For a LCA system that has m process, the size of the ECF vector will be Mx1. Total energy output (TEO) is obtained by dot product of the **f** vector and the EFC vector. TEO is computed by the equation shown in (3).

$$TEO = \sum_{i=0}^{M}(\mathbf{f}_i \,.\, \mathbf{ECF}_i) \quad (3)$$

m = Total number of processes defined in the LCA model

$\mathbf{f}_i$ = i^{th} element of the F vector

$\mathbf{ECF}_i$ = i^{th} element of the ECF vector

Total Waste Heat (TWH)

Waste Heat (WH) is defined only for primary energy conversion processes that converts a primary energy feedstock (like coal, natural gas etc) to a form of energy (like electricity) delivered as an output to meet the demand and also as intermediate inputs to other processes. For each primary energy Conversion Process (CP), Waste heat obtained by subtracting the output of the primary energy conversion process from the input primary energy feedstock to that primary energy conversion process as shown in equation (4).

$$Waste\ Heat_{CP,i} = Primary\ Energy\ Input_i - Energy\ Output_i \tag{4}$$

In matrix form, waste energy from all LCA processes is represented by a 1xM matrix, where M is the number of processes in the LCA model. Each element of the matrix is defined as shown in equation (5).

$$WH_{CP,i} = \begin{cases} QI_i * ECFI_i - QO_i * ECFO_i & \text{(For Energy Conversion Process)} \\ 0 & \text{(For other processes)} \end{cases} \tag{5}$$

QI_i is the quantity of the primary feedstock (like coal/natural gas). This physical unit of the primary feedstock is converted to MJ using an energy conversion factor $ECFI_i$ (e.g, MJ/kg). QO_i is the quantity of the output of the conversion process (like electricity). This unit is converted to MJ using another appropriate energy conversion factor $ECFO_i$ (e.g., MJ/kWh).

For non-conversion processes, the waste heat from non-electricity sources is added to the WH vector. For example, for the Aluminum extraction process, supplementary information of (Hertwich et al. 2015) specifies that the energy input is 4.5MJ/Kg. This is added to the WH vector for the Aluminum extraction process.

The total waste heat (TWH) in a given LCA system depends on the demand and is obtained by equation (6).

$$TWH = WH.s \tag{6}$$

Total Waste Heat from Feedstock (TWH_{FS})

Waste Heat from Feedstock is defined for every conversion process that takes a primary feedstock source as an input. In order to identify such conversion processes, a matrix FS is defined. FS is an Mx1 matrix and the definition of the elements of the matrix is shown in equation (7).

$$\mathbf{FS}_i = \begin{cases} 1 & \text{(For Energy Conversion Process)} \\ 0 & \text{(For other processes)} \end{cases} \tag{7}$$

For each conversion process that takes feedstock as an input, an Efficiency matrix is also defined. η is an Mx1 matrix and the definition of the elements of the matrix is shown in equation (8).

$$\eta_i = \begin{cases} \mathit{Efficiency} & \text{(For Energy Conversion Process)} \\ 0 & \text{(For other processes)} \end{cases} \tag{8}$$

Waste Heat from Feedstock (WH_{FS}) is the energy content from the feedstock that is dissipated as heat during the conversion process. WH_{FS} for every process is computed using equation (9).

$$\mathbf{WH}_{FS,i} = \begin{cases} 0 & (\text{if } \eta_i = 0) \\ \mathbf{f}_i * \mathbf{ECF}_i * \mathbf{FS}_i * \left(\left(\frac{1}{\eta_i}\right) - 1\right) & (\text{if } \eta_i > 0) \end{cases} \tag{9}$$

The waste heat from feedstock going directly to the energy output is a function of the energy carrier. However, the processes in the LCA model are setup such that, the primary conversion process (like process representing Coal to Electricity) is distinct from the “Final processes” (like process for electricity generation from Coal-IGCC) for a given subsystem-scale LCA model. The LCA assessment is performed by setting the demand of the “Final Process” ($\mathbf{f}_i$ for Final process) to a non-zero value (like 1 KWh). The value of the demand vector element for the conversion process ($\mathbf{f}_i$) is set to zero. In order to avoid the problem of zeroing-out the waste heat, $\mathbf{s}_i$ is used instead of $\mathbf{f}_i$. The input from the conversion process to the Final process is set to 1. Therefore, $\mathbf{s}_i$ of the conversion process will be equal to the $\mathbf{f}_i$ of the final process. Hence, equation is (9) is updated to use s_i instead of $\mathbf{f}_i$. Therefore, the Waste Heat from Feedstock (WH_{FS}) is computed using equation (10).

$$\mathbf{WH}_{FS,i} = \begin{cases} 0 & (\text{if } \eta_i = 0) \\ \mathbf{s}_i * \mathbf{ECF}_i * \mathbf{FS}_i * \left(\left(\frac{1}{\eta_i} \right) - 1 \right) & (\text{if } \eta_i > 0) \end{cases} \tag{10}$$

Total Waste Heat from Feedstock is the total waste heat from feedstock going directly to the output and is computed using equation (11).

$$TWH_{FS} = \sum_{i=0}^{M} WH_{FS,i} \tag{11}$$

Net Energy Ratio (NER)

NER is defined as the ratio of the net energy produced as output, which is represented as Total Energy Output to the Total Waste Heat produced during generation. NER is computed using the equation (12).

$$NER = \frac{Total\ Energy\ Output\ (TEO)}{Total\ Waste\ Heat\ (TWH)} \tag{12}$$

Gross Energy Ratio (GER)

GER is defined as the gross energy extracted to the total waste energy produced during generation. The gross energy is defined as the sum of the total energy produced for output (TED) and the Total Waste Energy produced during generation. GER is computed using the equation (13).

$$GER = \frac{Total\ Energy\ Output + Total\ Waste\ Energy}{Total\ Waste\ Energy} \tag{13}$$

Net External Energy Ratio (NEER)

NEER is a measure of net energy generation without considering energy content of feedstock as an intermediate energy input that is converted to heat as a component of Total Waste Heat. The NEER is computed using equation (14). The Total Waste Heat from Feedstock represents the energy content in the primary feedstock (like coal) that is converted to an output in Total Energy Output. This is subtracted from the Total Waste Energy to obtain the total external energy required to meet the energy demand.

$$NEER = \frac{Total\ Energy\ Output}{(Total\ Waste\ Heat - Total\ Waste\ Heat\ from\ Feedstock\ going\ directly\ to\ output)} \tag{14}$$

Gross External Energy Ratio (GEER)

GEER is a measure of gross energy generation without taking feedstock into consideration. The GEER is computed using equation (15).

$$GEER = \frac{(Total\ Energy\ Output + Total\ Waste\ Energy - Total\ Waste\ Heat\ from\ Feedstock\ going\ directly\ to\ output)}{(Total\ Waste\ Energy - Total\ Waste\ Heat\ from\ Feedstock\ going\ directly\ to\ output)} \tag{15}$$

Method 2: NER and NEER from CED

ERR is computed using the (Arvesen and Hertwich 2015) method for electricity generation technologies using the data from (Hertwich et al. 2015). The NER and NEER are calculated from CED using equations (16) and (17) respectively. (Arvesen and Hertwich 2015) state that the when energy ratios are calculated the denominator should contain the energy that is diverted from the society. Energy lost from sources like fugitive emissions cannot be considered as energy diverted from the society. However, CED represents the total energy extracted from nature. The energy lost from sources that cannot be considered as diverted from the society should therefore be subtracted from the CED. The Energy Output, Fuel Input and Energy lost are computed using the data in the LCA models and is described in the future sections of this chapter. The CED is used from the results of the study in (Hertwich et al. 2015).

$$NER = \frac{Energy\ Output}{CED} \tag{16}$$

$$NEER = \frac{Energy\ Output}{CED - (Fuel\ Input + Energy\ lost)} \tag{17}$$

We consider the LCA model for electricity generation from Coal without IGCC, that we have developed using data from (Hertwich et al. 2015), as an example to compute NER and NEER. Figure 1 shows a part of the LCA model showing processes that contributes to the “Energy lost” and also the “fuel input”. The “Plant Operation” process is the process that represents conversion of coal to electricity.

The total fuel input is calculated using equation (18). Waste Heat$_{PO}$ represents the waste heat released by the "Plant Operation" process. Energy Output$_{PO}$ represents the energy output from the "Plant Operation" process. (Arvesen and Hertwich 2015) state that in order to be consistent, all the factors that make up the energy return ratio should be in the same heat values unit. From the model, the waste heat of 4.938MJ is released per kWh (Energy Output = 3.6 MJ) of electricity from the "Plant Operation" process. Assuming that the waste heat is already in the HHV (High Heating Value), the Energy Output is converted to HHV from LHV (Low Heating Value) by increasing it by 5%.

$$Fuel\ Input = Waste\ Heat_{PO} + Energy\ Output_{PO} \qquad (18)$$

$$Fuel\ Input = 4.938 + (3.6 * 1.05)\ \text{MJ} \qquad (19)$$

The Energy lost from equation (17) is calculated by adding the energy lost by methane emissions from the "Plant Operation" process and the "Coal Transport" process. It is calculated by using equations (20) and (21)

$$Methane_{kg} = (1KWh\ \times (1.03 \times 10^{-5})kg/KWh) + (0.3149kg\ \times (8.55 \times 10^{-5})kg/kg) \qquad (20)$$

$$Energy\ lost = Methane_{kg} \times HHV\ of\ methane \qquad (21)$$

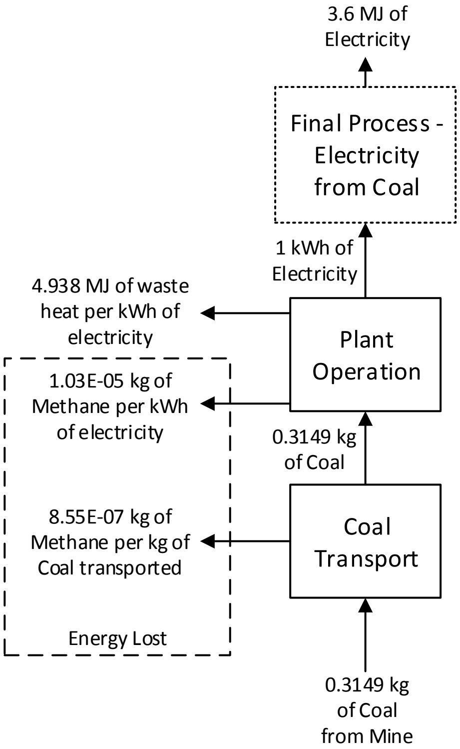


Figure 1: Part of the Coal without IGCC Model showing fuel input & methane emissions

OPEN SOURCE

One of the goals of the thesis is to enable expansion of system-scale LCA model. The expansion can be achieved by adding data and processes to the **A** and the **B** matrices of the system-scale LCA model.

The open source methodology also enables development of any subsystem-scale and system-scale LCA models. This goal is achieved by incorporating these design principles in the methodology –

1. The process attributes are designed to be generic and they can be used to represent any process uniquely.
2. There are no size limitations to the A and B matrices.

3. The process of adding data or new processes to existing LCA models is designed to be straightforward and simple and is explained in the Implementation chapter.

4. The merging algorithm that is used to merge subsystem-scale models into a system-scale LCA model is designed to be generic. Any number of models can be merged using the algorithm and there is no restriction on the number of processes or types of processes.

Implementation

LCA DATA

Data from the (Hertwich et al. 2015) is used to develop the LCA models in this thesis. (Hertwich et al. 2015) sub-divided into 21 subsystem-scale technology files (Microsoft Excel Workbook), each technology file representing a different electricity generation technology. The data for the following 21 electricity generation technologies are used –

1. COAL, with IGCC
2. COAL, without IGCC
3. COAL, subcritical with CCS
4. COAL, subcritical without CCS
5. COAL, supercritical with CCS
6. COAL, supercritical without CCS
7. CSP, trough wet-mined syn
8. GAS, NGCC with CCS
9. GAS, NGCC without CCS
10. HYDRO, dam storage, Baker 1 (Aysen)
11. HYDRO, dam storage, Baker 2 (Aysen)
12. PV, CdTe, ground-mounted
13. PV, CdTe, roof-mounted

14. PV, CIGS, ground-mounted
15. PV, CIGS, roof-mounted
16. PV, poly-Si, ground-mounted
17. PV, poly-Si, roof-mounted
18. CSP, central tower dry
19. WIND, offshore, gravity-based foundation
20. WIND, offshore, steel foundation
21. WIND, onshore

Each file contains processes defined for a particular electricity generation technology. Each process is defined as a different spreadsheet in the workbook. Each process contains inputs from numerous other processes. The processes that input into a given process are categorized into different types depending on the source of the data –

1. Own System: These are processes provide some input to a given process and are defined in same LCA model.
2. Ecoinvent: These are processes provide some input to a given process but are taken from Ecoinvent database. The ecoinvent processes are not defined in the technology file. Access to the ecoinvent database is required in order to get the definition of the processes to complete the LCA model.
3. Input-Output Background: These processes mostly represent capital investment related processes.

4. Natural resources: These processes represent the natural resource use like water and land use. They do not include primary energy natural resources like coal, natural gas etc.

5. Emissions: These processes represent emissions like CO2, NO2, VOC, Particulate matter etc

SOFTWARE TOOLS

Matlab is used to develop the LCA system-scale model and perform LCA assessment on the models. Object oriented Matlab is used to implement the definition of processes and all code related to parsing the technology files, creation of matrices, merging subsystem-scale matrices into system-scale matrices and performing net-energy analysis on the LCA models.

CREATING SYSTEM-SCALE LCA MODEL

The system-scale LCA model is created using the following two steps –

1. The individual technology files (that contain data for subsystems) are parsed and subsystem-scale LCA models are created. Subsystem-scale LCA models contain A header-matrix pair, B header-matrix pair and F matrix.

2. The subsystem-scale LCA models are then merged to create a system-scale LCA model.

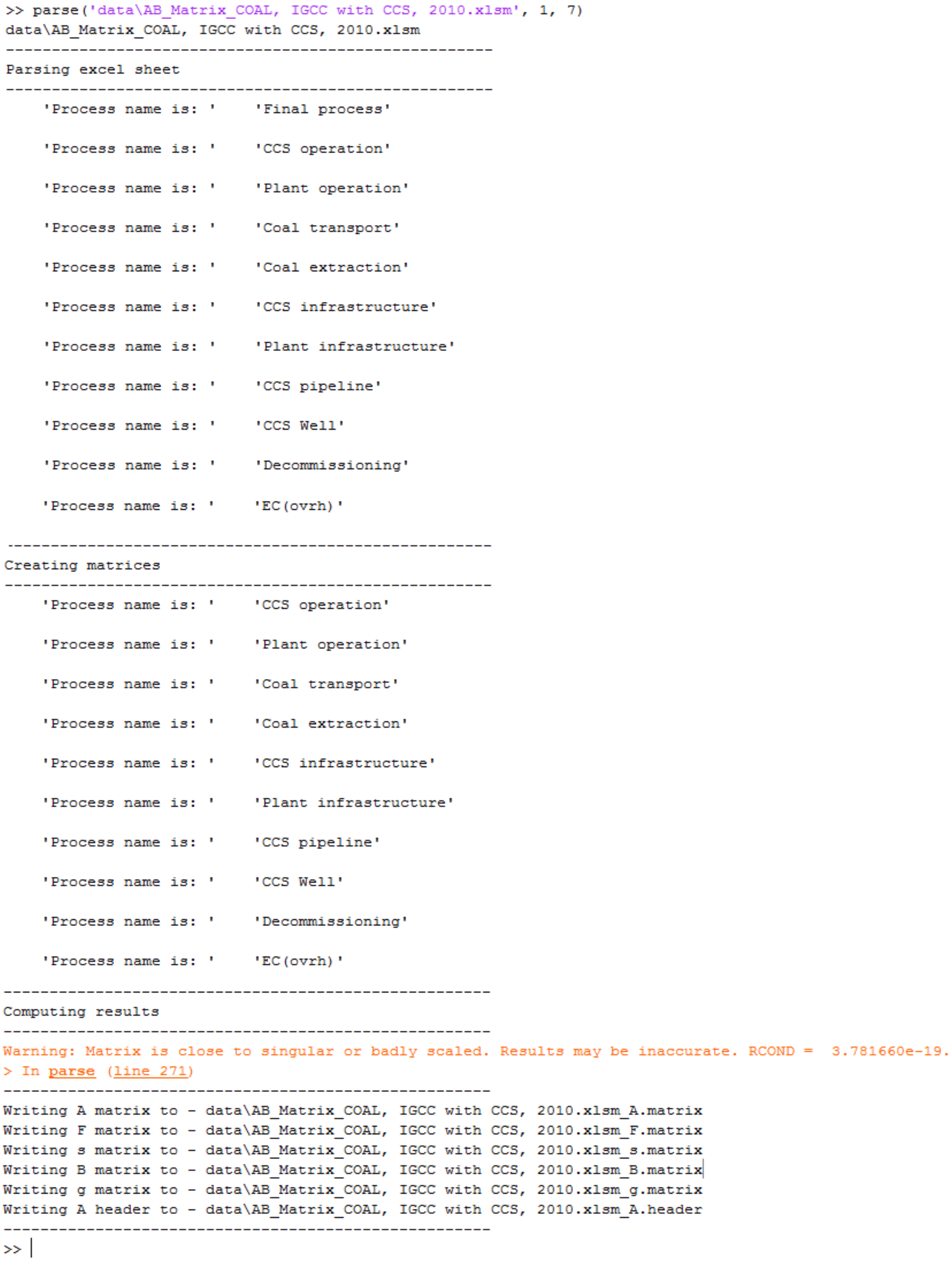
Creating subsystem-scale LCA models

A Matlab program called “parse” is developed and is used to create the subsystem-scale LCA model for every technology. This program takes the technology workbook file as an input and produces the A header, **A** matrix, **B** header, **B** matrix and the **f** vector.

The following functionality is implemented in this program –

1. A number of spreadsheets in the excel workbook is read. This will represent the number of "Own-system" processes to be created for the subsystem.
2. Each spreadsheet is read and a process object is created. All the attributes of the process object is populated using the data in the sheet. Child processes are also created for every process that provides an input to the process under consideration.
3. After all the spreadsheets are read, the model will have a structure as shown in Figure 29.
4. The A header and **A** matrix are created by inserting data from all the processes and their children.
5. The B header and **B** matrix are created by inserting data from all the processes.
6. A preliminary **f** vector is created by setting the demand for the electricity to 1 kWh.
7. The A header, **A** matrix, B header, **B** matrix and **f** vector are created as separate CSV files.

Figure 2 shows an example of how the "parse" program is run in Matlab taking a Microsoft Excel workbook file that represents one electricity generation technology. This file is obtained as part of the data from (Hertwich et al. 2015).



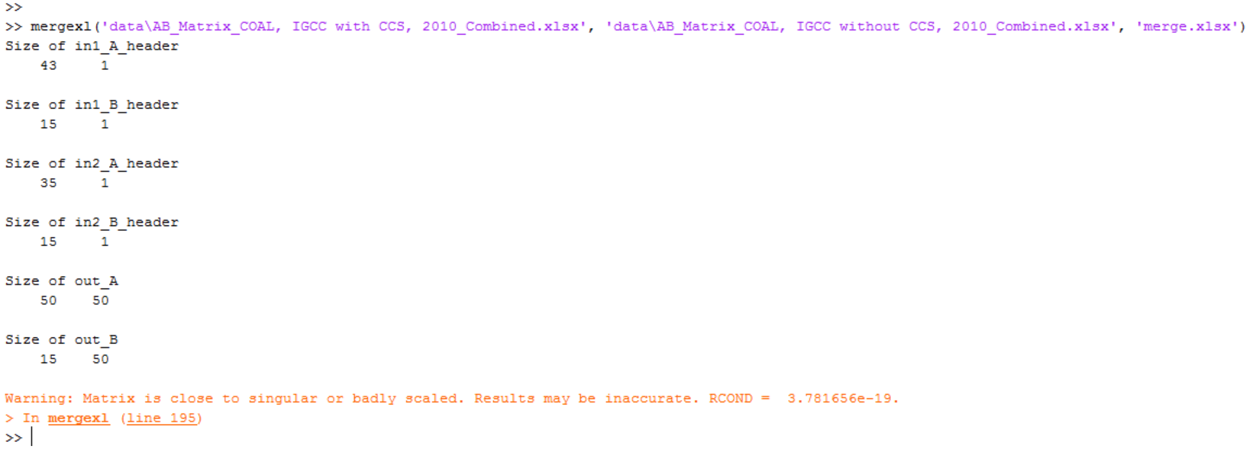
```
>> parse('data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm', 1, 7)
data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm
-----------------------------------------------------
Parsing excel sheet
-----------------------------------------------------
    'Process name is: '    'Final process'

    'Process name is: '    'CCS operation'

    'Process name is: '    'Plant operation'

    'Process name is: '    'Coal transport'

    'Process name is: '    'Coal extraction'

    'Process name is: '    'CCS infrastructure'

    'Process name is: '    'Plant infrastructure'

    'Process name is: '    'CCS pipeline'

    'Process name is: '    'CCS Well'

    'Process name is: '    'Decommissioning'

    'Process name is: '    'EC(ovrh)'

-----------------------------------------------------
Creating matrices
-----------------------------------------------------
    'Process name is: '    'CCS operation'

    'Process name is: '    'Plant operation'

    'Process name is: '    'Coal transport'

    'Process name is: '    'Coal extraction'

    'Process name is: '    'CCS infrastructure'

    'Process name is: '    'Plant infrastructure'

    'Process name is: '    'CCS pipeline'

    'Process name is: '    'CCS Well'

    'Process name is: '    'Decommissioning'

    'Process name is: '    'EC(ovrh)'

-----------------------------------------------------
Computing results
-----------------------------------------------------
Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND =  3.781660e-19.
> In parse (line 271)
-----------------------------------------------------
Writing A matrix to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_A.matrix
Writing F matrix to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_F.matrix
Writing s matrix to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_s.matrix
Writing B matrix to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_B.matrix
Writing g matrix to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_g.matrix
Writing A header to - data\AB_Matrix_COAL, IGCC with CCS, 2010.xlsm_A.header
-----------------------------------------------------
>> |
```

Figure 2: Execution of Parse program in Matlab

The technology files are Microsoft Excel workbooks that use Visual Basic Macros. Some of the technology files were not readable by Matlab R2015 on Windows 7. Such files could only be read using Matlab R2015 on Apple iOS. However, Matlab running on Apple iOS does not support creation and insertion of individual sheets in an Excel workbook. While it would have been desirable for the "parse" program to create an Excel workbook with separate spreadsheets for A header, **A** matrix, B header, **B** matrix and the **f** vector, this was not possible due to the two problems above. Therefore, the "parse" program is designed to write the matrices and headers into CSV files. These CSV files are combined into a single Microsoft Excel workbook manually in order to use the "merge" program.

Merging subsystem-scale LCA models

The "mergexl" program is used to merge two subsystem-scale LCA models. It takes two input subsystem-scale LCA models in the form of Microsoft Excel Workbooks and produces a merged output Microsoft Excel Workbook. Figure 3 shows an example of how the "mergexl" program is run in Matlab.



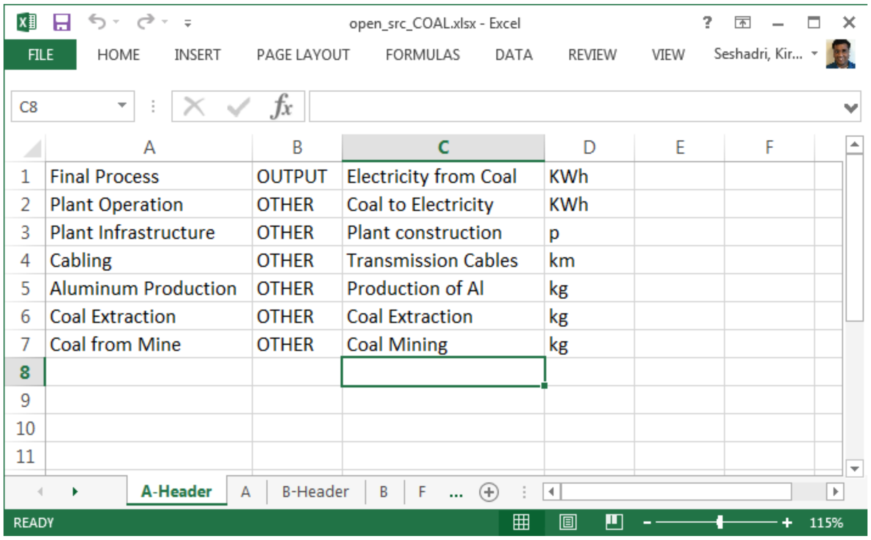
```
>>
>> mergexl('data\AB_Matrix_COAL, IGCC with CCS, 2010_Combined.xlsx', 'data\AB_Matrix_COAL, IGCC without CCS, 2010_Combined.xlsx', 'merge.xlsx')
Size of in1_A_header
    43     1

Size of in1_B_header
    15     1

Size of in2_A_header
    35     1

Size of in2_B_header
    15     1

Size of out_A
    50    50

Size of out_B
    15    50

Warning: Matrix is close to singular or badly scaled. Results may be inaccurate. RCOND =  3.781656e-19.
> In mergexl (line 195)
>> |
```

Figure 3: Execution of Merge Program in Matlab

All the 21 subsystem-scale LCA models are merged taking two at a time as shown in Figure 35.

SYSTEM-SCALE AND SUBSYSTEM-SCALE LCA ASSESSMENT

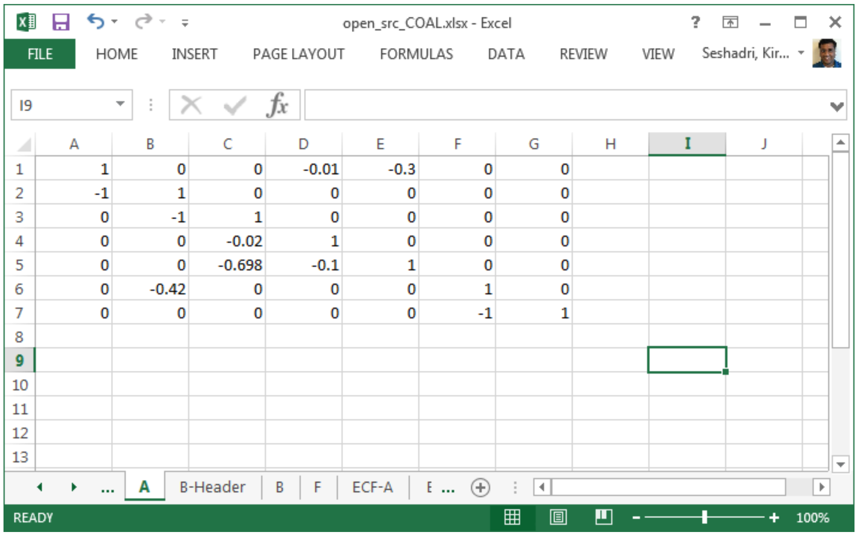
A Matlab program called “lca_comp” is developed that will take two Microsoft Excel Workbooks as an input. The first Excel Workbook contains the LCA model (mainly **A** and **B** matrices). The second Excel Workbook contains the demand vector (F vector). Figure 4 shows an example of an A header of a LCA model that represents the generation of electricity from coal shown in Figure 28. The A header contains the attributes of the processes in the **A** matrix. Because the **A** matrix is a square matrix, the A-header represents the processes in both the X and Y direction. Each row of the A header represents a process and the cells of the row represent the attributes of the process.



	A	B	C	D	E	F
1	Final Process	OUTPUT	Electricity from Coal	KWh		
2	Plant Operation	OTHER	Coal to Electricity	KWh		
3	Plant Infrastructure	OTHER	Plant construction	p		
4	Cabling	OTHER	Transmission Cables	km		
5	Aluminum Production	OTHER	Production of Al	kg		
6	Coal Extraction	OTHER	Coal Extraction	kg		
7	Coal from Mine	OTHER	Coal Mining	kg		
8						
9						
10						
11						

Figure 4: An example of an A-Header worksheet

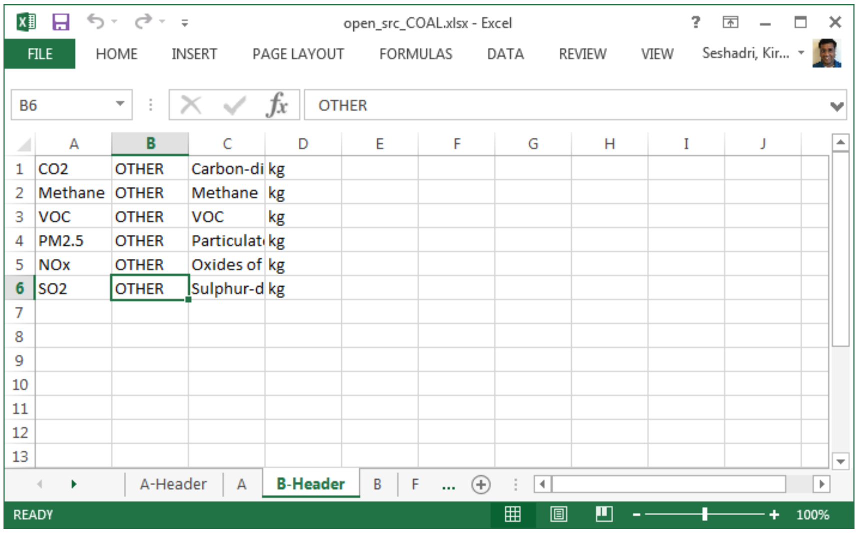
Figure 5 shows an example of an A matrix of the LCA model that represents electricity generation from Coal. It contains the actual **A** matrix with processes as defined by the A header.



	A	B	C	D	E	F	G
1	1	0	0	-0.01	-0.3	0	0
2	-1	1	0	0	0	0	0
3	0	-1	1	0	0	0	0
4	0	0	-0.02	1	0	0	0
5	0	0	-0.698	-0.1	1	0	0
6	0	-0.42	0	0	0	1	0
7	0	0	0	0	0	-1	1

Figure 5: An example of an **A** matrix worksheet

Figure 6 shows an example of the B header of the LCA model that represents electricity generation from Coal. The B header contains the attributes of the processes in the B matrix. Each row in the B header list represents an emissions or a waste heat process. In the X direction, every column of the **B** matrix is represented by the processes in the A header list.

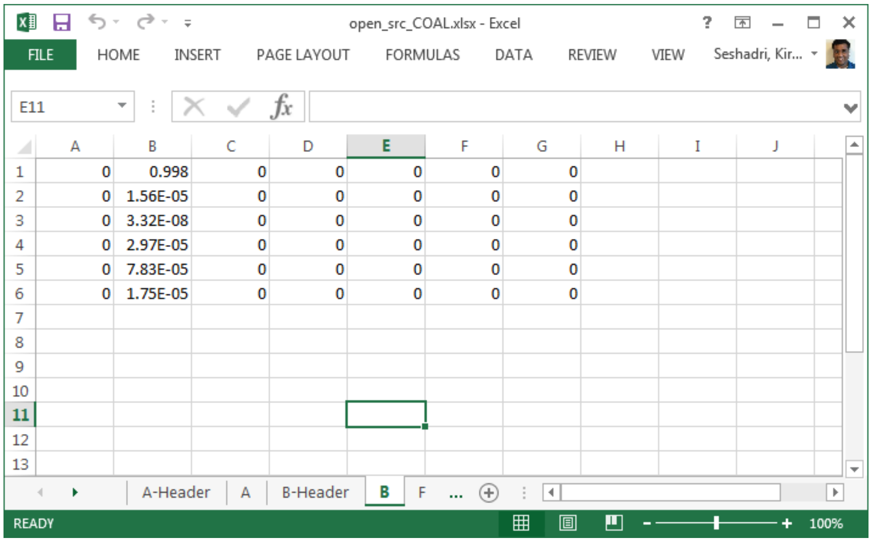


B6 OTHER

	A	B	C	D	E	F	G	H	I	J
1	CO2	OTHER	Carbon-di	kg						
2	Methane	OTHER	Methane	kg						
3	VOC	OTHER	VOC	kg						
4	PM2.5	OTHER	Particulat	kg						
5	NOx	OTHER	Oxides of	kg						
6	SO2	OTHER	Sulphur-d	kg						
7										
8										
9										
10										
11										
12										
13										

Figure 6: An example of a B Header

Figure 7 shows an example of the B matrix in the LCA model. It contains the actual **B** matrix.

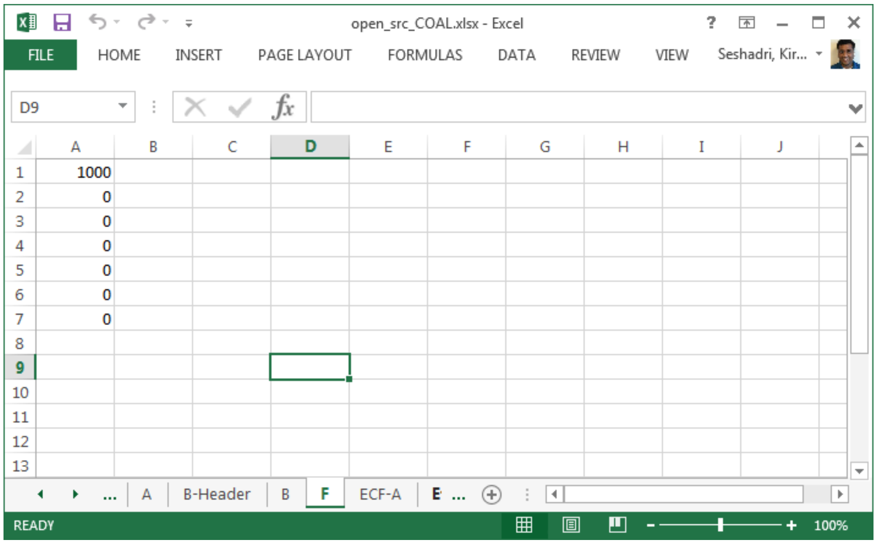


E11

	A	B	C	D	E	F	G	H	I	J
1	0	0.998	0	0	0	0	0			
2	0	1.56E-05	0	0	0	0	0			
3	0	3.32E-08	0	0	0	0	0			
4	0	2.97E-05	0	0	0	0	0			
5	0	7.83E-05	0	0	0	0	0			
6	0	1.75E-05	0	0	0	0	0			
7										
8										
9										
10										
11										
12										
13										

Figure 7: An example of the **B** matrix

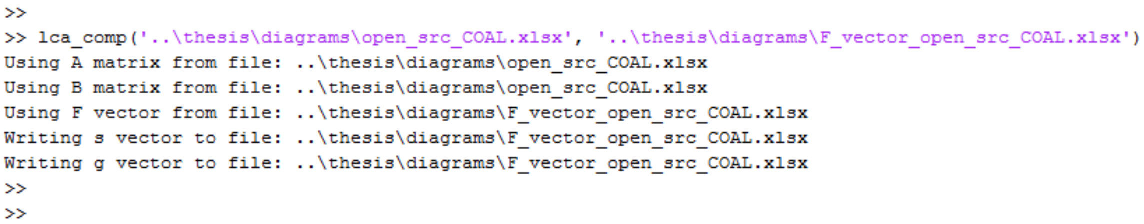
Figure 8 shows an example of the **f** vector of the LCA model that represents electricity generation from Coal. The **f** vector contains only one element per row and it represents the demand for the output of the corresponding process in the same row of the A header.



	A	B	C	D	E	F	G	H	I	J
1	1000									
2	0									
3	0									
4	0									
5	0									
6	0									
7	0									
8										
9										
10										
11										
12										
13										

Figure 8: An example of the **f** vector

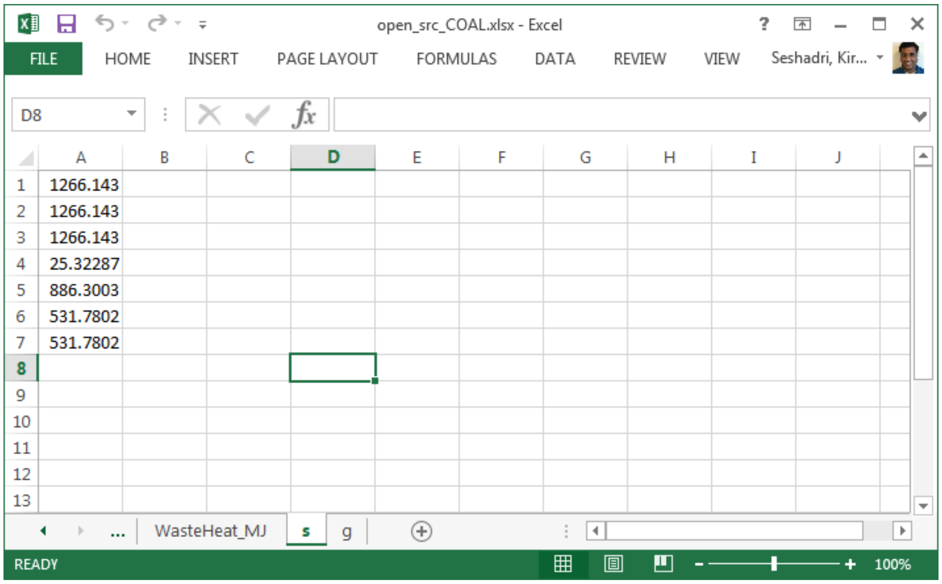
The “lca_comp” program is run and it will generate the s-matrix and the g-matrix. These matrices are written into the same Microsoft Excel Workbook as new worksheets. Figure 9 shows how the “lca_comp” is run using Matlab.



```
>>
>> lca_comp('..\thesis\diagrams\open_src_COAL.xlsx', '..\thesis\diagrams\F_vector_open_src_COAL.xlsx')
Using A matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using B matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using F vector from file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Writing s vector to file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Writing g vector to file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
>>
>>
```

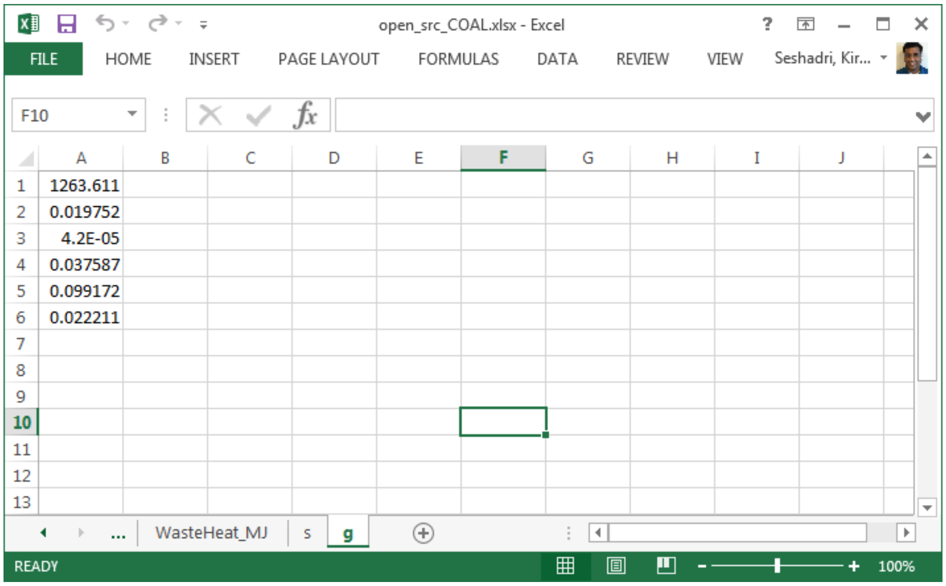
Figure 9: LCA Assessment program execution in Matlab

Figure 10 and Figure 11 show the **s** and the **g** vectors that are written into the same Excel Workbook that contains the **f** vector, after LCA assessment.



	A
1	1266.143
2	1266.143
3	1266.143
4	25.32287
5	886.3003
6	531.7802
7	531.7802

Figure 10: An example of the s vector



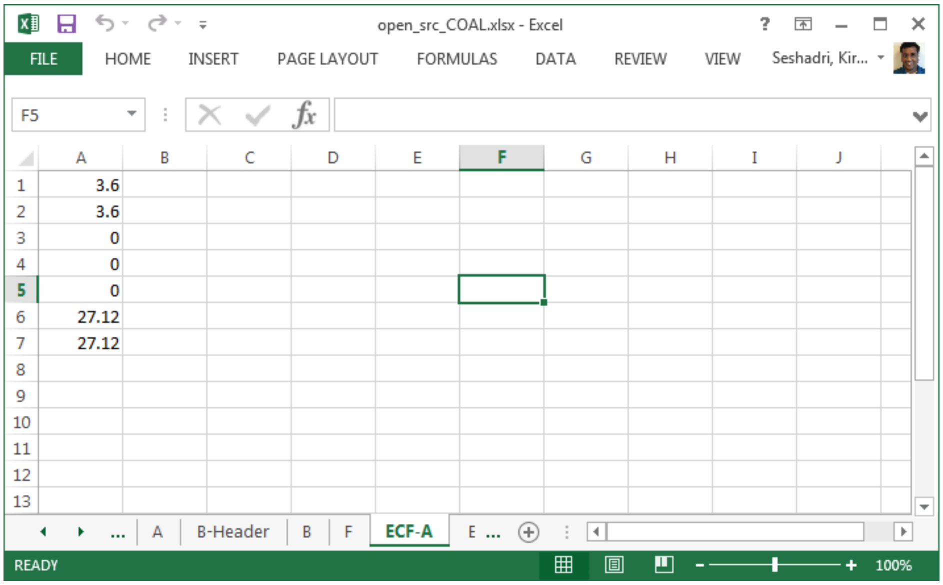
	A
1	1263.611
2	0.019752
3	4.2E-05
4	0.037587
5	0.099172
6	0.022211

Figure 11: An example of the g vector

SYSTEM-SCALE AND SUBSYSTEM-SCALE ENERGY RETURN RATIOS

A Matlab program “err_comp” is developed to compute the energy return ratios. In addition to the A, B and F matrices (like lca_comp), the program reads four matrices – ECF-A, Feedstock, Efficiency and WasteHeat_MJ matrices. The description of these matrices are provided further in this chapter. The matrices are input to the program using three input arguments. The first argument is the Microsoft Excel Workbook containing the LCA model that comprises of the A, B, ECF-A, Efficiency and WasteHeat_MJ matrices. This is the second input argument to the program is the Excel workbook that contains the F vector. The third argument to the program is the Excel workbook that contains the “Feedstock” vector.

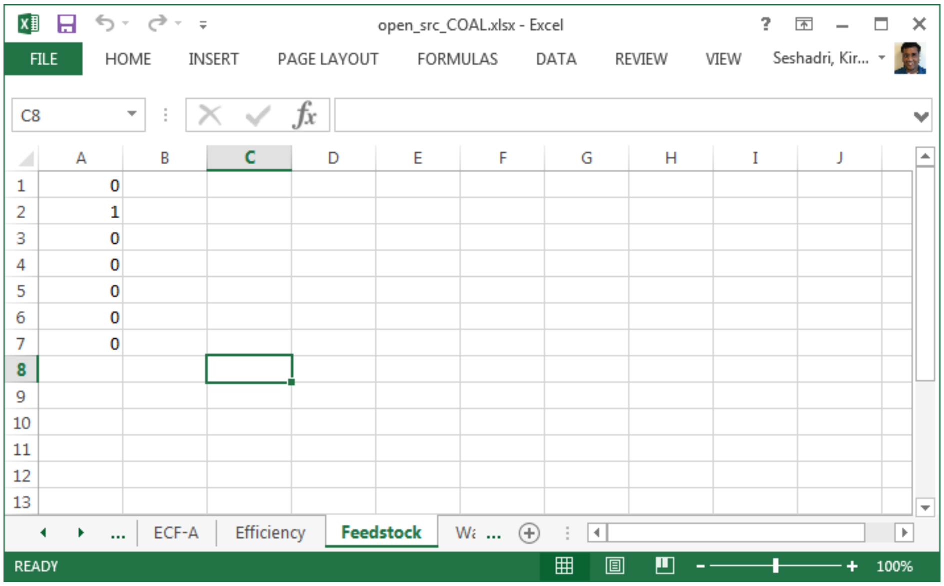
The Energy Conversion Matrix (ECF-A) contains the energy conversion factors to MJ for each row in **A**. Figure 12 shows an example of the ECF-A matrix of the LCA model that represents electricity generation from Coal.



	A
1	3.6
2	3.6
3	0
4	0
5	0
6	27.12
7	27.12

Figure 12: An example of the Energy Conversion Factor vector

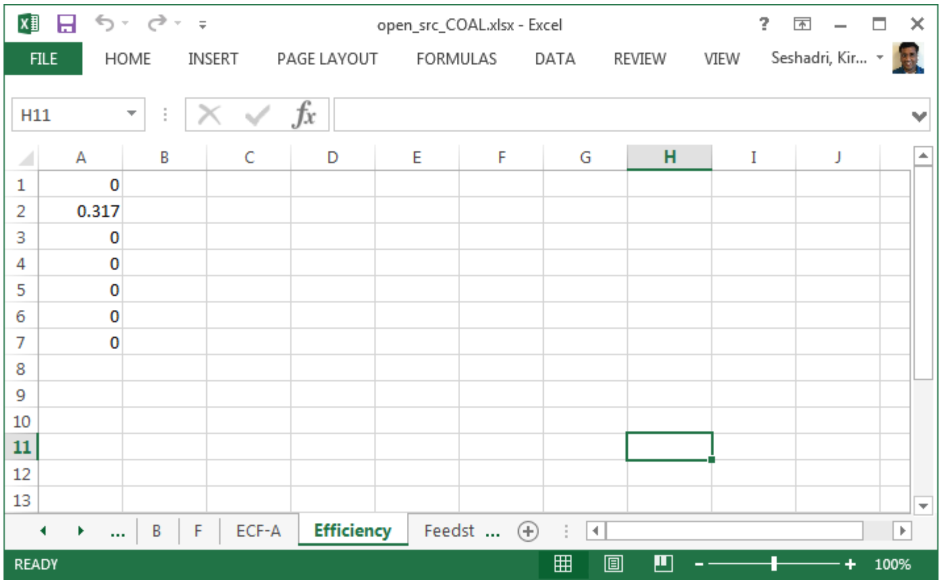
The Feedstock (FS) matrix is used to identify processes that represent primary conversion of fuel under consideration to electricity. Figure 13 shows the FS matrix of the LCA model that represents electricity generation from Coal. This is provided as an input to the err_comp program in order to provide the flexibility to the user to decide what is considered as feedstock and what is not. For example, when analyzing the electricity generation from Coal, Natural gas should not be considered as feedstock but Coal should be considered as feedstock, for the purposes of NEER and GEER calculations. Similarly, when analyzing the electricity generation from Wind, Coal and Natural gas should not be considered as feedstock. By making this an argument to the err_comp program, the methodology provides the flexibility of identifying what fuel sources are considered as feedstock and what is not.



	A
1	0
2	1
3	0
4	0
5	0
6	0
7	0

Figure 13: An example of Feedstock vector

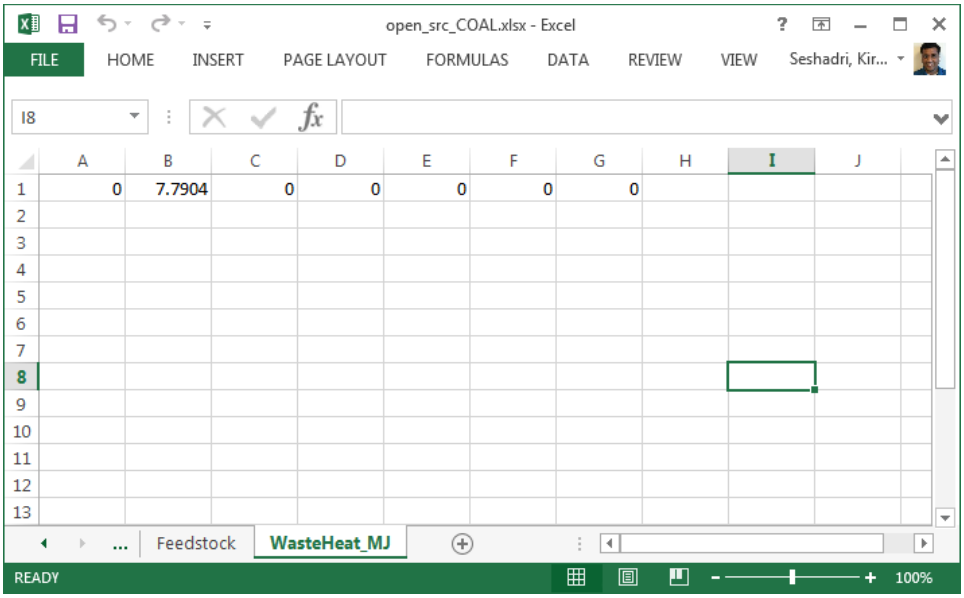
The Efficiency matrix contains the efficiency for primary energy conversion processes. Figure 14 shows an example of the Efficiency matrix of the LCA model that represents electricity generation from Coal.



	A
1	0
2	0.317
3	0
4	0
5	0
6	0
7	0

Figure 14: An example of Efficiency vector

The WasteHeat_MJ matrix represents the Waste Energy for every conversion process computed as described in Total Waste Heat (TWH). The entries of the WasteHeat_MJ matrix is in unit Mega Joules. Figure 15 shows an example of the Waste Energy matrix of the LCA model that represents electricity generation from Coal.



	A	B	C	D	E	F	G
1	0	7.7904	0	0	0	0	0

Figure 15: An example of the Waste Heat vector

The Matlab program “err_comp” computes the energy return ratios by reading the Microsoft Excel Workbook that contains the integrated LCA models that includes all electricity generation technologies. The program computes all the energy return ratios NER, NEER, GER and NEER using methodology described in Energy Return Ratios. It also reports Total Energy Output, Total Waste Heat and Total Waste Heat from Feedstock. Figure 16 shows how the “err_comp” is executed in Matlab.

A Matlab program “lca_err_comp” performs both functions viz. LCA analysis and ERR computation. The arguments of the “lca_err_comp” program are the same as “err_comp”. This program calls lca_comp() first and then calls err_comp(). This program is created as a convenience program to perform LCA analysis and ERR computation by a single program. Figure 17 shows how the lca_comp_err program is executed in Matlab.

```
>> err_comp('..\thesis\diagrams\open_src_COAL.xlsx', '..\thesis\diagrams\F_vector_open_src_COAL.xlsx', '..\thesis\diagrams\FS_vector_open_src_COAL.xlsx')
Using A matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using F vector from file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Using ECF vector from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using FS vector from file: ..\thesis\diagrams\FS_vector_open_src_COAL.xlsx
Using WasteHeat_MJ vector from file: ..\thesis\diagrams\open_src_COAL.xlsx
Total_WasteHeat_MJ =
   9.8638e+03

Total_EnergyOut_MJ =
        3600

Total_WasteHeat_from_Feedstock_MJ =
   9.8208e+03

NER =
    0.3650

GER =
    1.3650

NEER =
   83.7907

GEER =
   84.7907

>>
```

Figure 16: Execution of Energy return ratio computation program in Matlab

```
>>
>> lca_err_comp('..\thesis\diagrams\open_src_COAL.xlsx', '..\thesis\diagrams\F_vector_open_src_COAL.xlsx', '..\thesis\diagrams\FS_vector_open_src_COAL.xlsx')
-----------------------------------------
--------- Running LCA Analysis ----------
-----------------------------------------
Using A matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using B matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using F vector from file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Writing s vector to file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Writing g vector to file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
------------------------------------------------
--------- Running Net Energy Analysis ----------
------------------------------------------------
Using A matrix from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using F vector from file: ..\thesis\diagrams\F_vector_open_src_COAL.xlsx
Using ECF vector from file: ..\thesis\diagrams\open_src_COAL.xlsx
Using FS vector from file: ..\thesis\diagrams\FS_vector_open_src_COAL.xlsx
Using WasteHeat_MJ vector from file: ..\thesis\diagrams\open_src_COAL.xlsx
Total_WasteHeat_MJ =
   9.8638e+03

Total_EnergyOut_MJ =
        3600

Total_WasteHeat_from_Feedstock_MJ =
   9.8208e+03

NER =
    0.3650

GER =
    1.3650

NEER =
   83.7907

GEER =
   84.7907

>>
```

Figure 17: Execution of the lca_err_comp program in Matlab

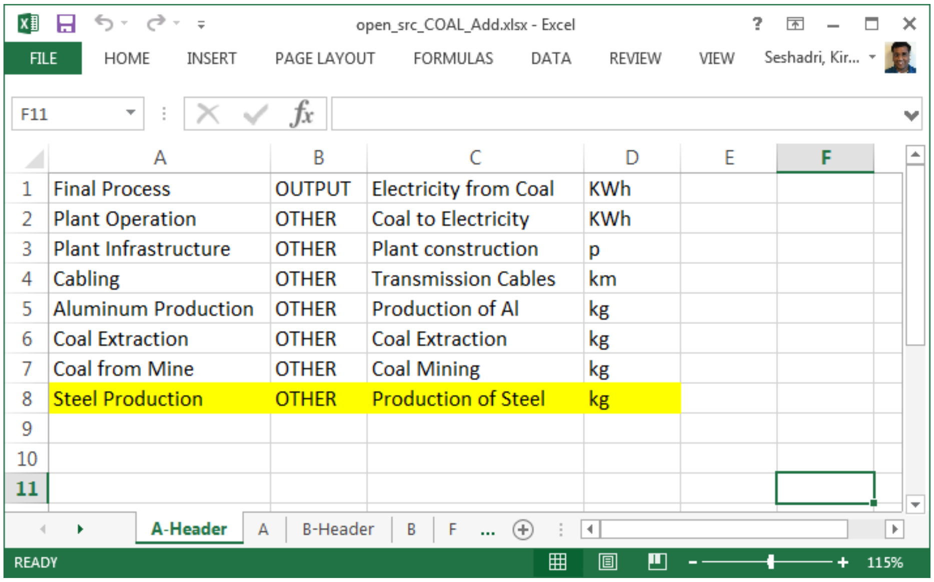
OPEN SOURCE

Open source methodology enables development of any LCA subsystem-scale and system-scale models. In addition, the open source methodology also enables the expansion of the merged system-scale LCA model by adding processes to the LCA model.

Expansion of LCA models by adding processes

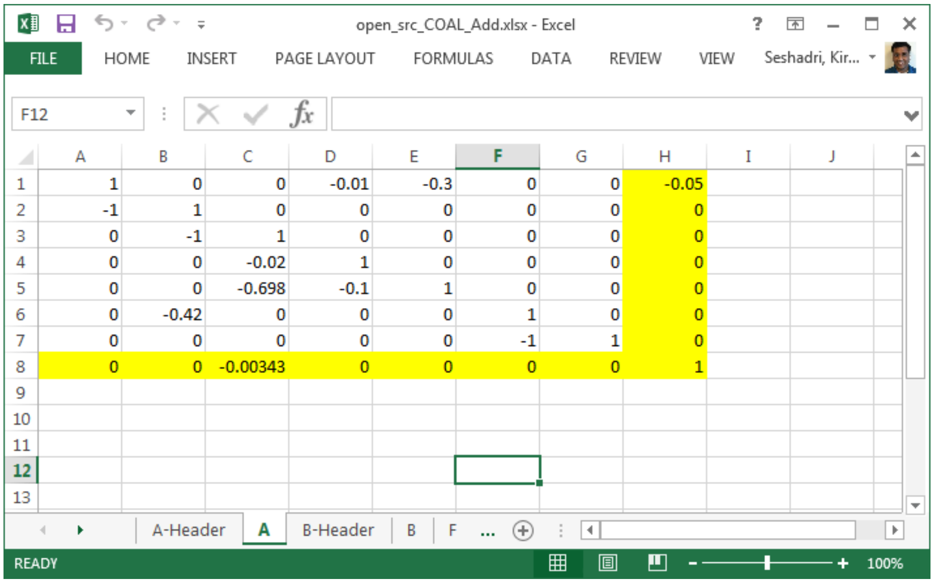
The subsystem-scale or system-scale LCA models are expanded by adding processes to the A and/or B header-matrix pairs. Processes can be added by simply adding rows and columns to the “A-Header”, “A-matrix”, “B-Header” or “B-matrix” worksheets of the Microsoft Excel workbook that contains the LCA model. Related changed to the **f** vector will be required before performing LCA assessment or ERR computation.

An example LCA model for generation of electricity from coal is shown in Figure 28. In order to add a process that represents use of steel to the LCA model, a new row is added to the A-Header. Figure 18 shows the highlighted row that represents process of steel generation. To restrict the scope of the model, the process of steel generation is defined to output 1 kg of steel. Additionally, it is defined to consume some amount of electricity to produce. Lastly, the “Plant infrastructure” process is modified to have a steel input. These inputs and outputs to the steel generation process is represented in the A-matrix. The additions to the A-matrix are shown in Figure 19 as highlighted cells. The emissions related to the steel generation process are added to the B-matrix as shown in Figure 20 as highlighted cells. The demand F-matrix is also modified to account of the new process that is added as shown in Figure 21 as a highlighted cell. If energy return ratios have to be computed, the matrices required for ERR computation should also be accordingly modified.



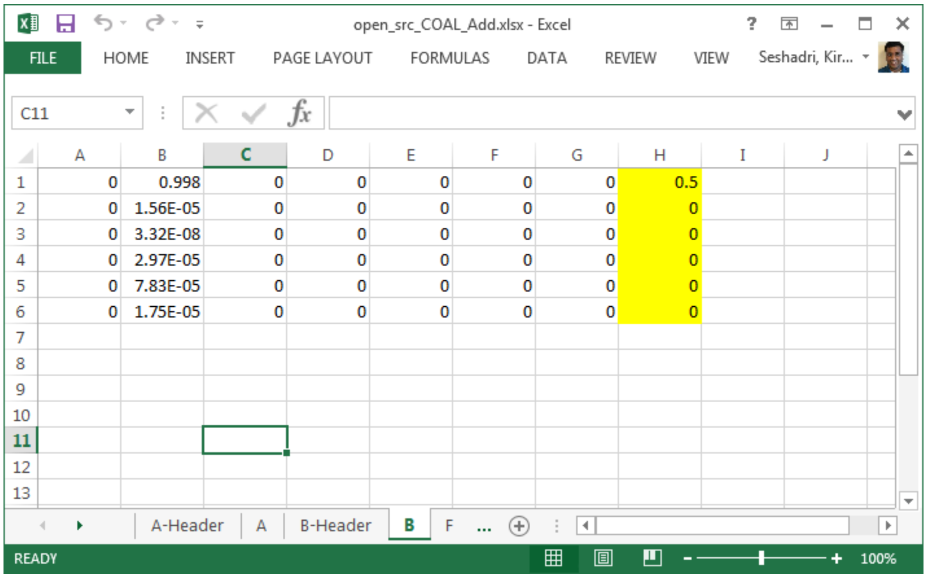
	A	B	C	D	E	F
1	Final Process	OUTPUT	Electricity from Coal	KWh		
2	Plant Operation	OTHER	Coal to Electricity	KWh		
3	Plant Infrastructure	OTHER	Plant construction	p		
4	Cabling	OTHER	Transmission Cables	km		
5	Aluminum Production	OTHER	Production of Al	kg		
6	Coal Extraction	OTHER	Coal Extraction	kg		
7	Coal from Mine	OTHER	Coal Mining	kg		
8	Steel Production	OTHER	Production of Steel	kg		

Figure 18: Addition of a process to the A-Header



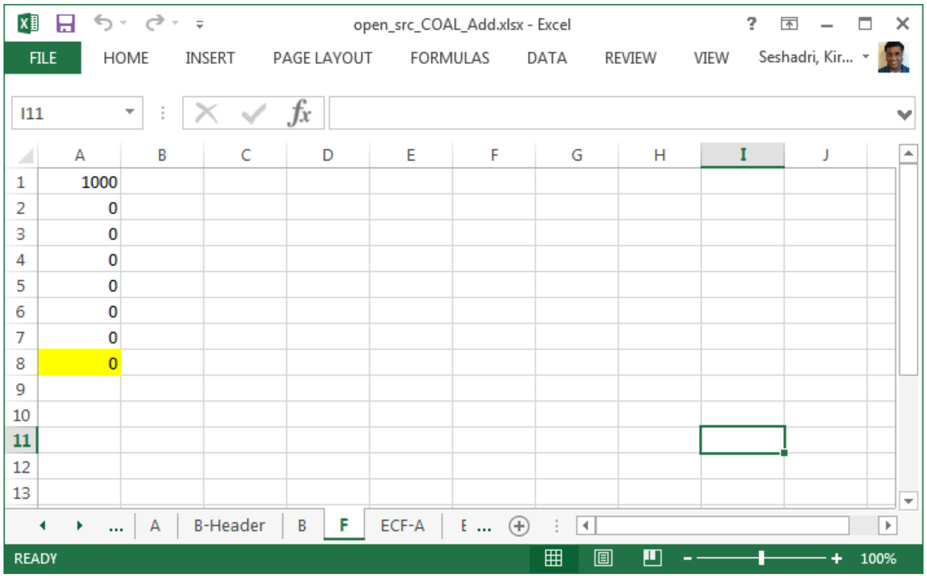
	A	B	C	D	E	F	G	H
1	1	0	0	-0.01	-0.3	0	0	-0.05
2	-1	1	0	0	0	0	0	0
3	0	-1	1	0	0	0	0	0
4	0	0	-0.02	1	0	0	0	0
5	0	0	-0.698	-0.1	1	0	0	0
6	0	-0.42	0	0	0	1	0	0
7	0	0	0	0	0	-1	1	0
8	0	0	-0.00343	0	0	0	0	1

Figure 19: Addition of a process to A-matrix



	A	B	C	D	E	F	G	H	I	J
1	0	0.998	0	0	0	0	0	0.5		
2	0	1.56E-05	0	0	0	0	0	0		
3	0	3.32E-08	0	0	0	0	0	0		
4	0	2.97E-05	0	0	0	0	0	0		
5	0	7.83E-05	0	0	0	0	0	0		
6	0	1.75E-05	0	0	0	0	0	0		
7										
8										
9										
10										
11										
12										
13										

Figure 20: Addition of a process to B-matrix



	A	B	C	D	E	F	G	H	I	J
1	1000									
2	0									
3	0									
4	0									
5	0									
6	0									
7	0									
8	0									
9										
10										
11										
12										
13										

Figure 21: Addition of process to F vector

Development of any subsystem-scale and system-scale LCA models

A generic definition of the “process” class is created to be used to represent any arbitrary process. A number of customizations that was performed for the “process” class used for developing LCA models from (Hertwich et al. 2015) data is removed to create the open-source class definition of the "process". The members of the open-source version of the "process" class are made generic and the methods are simplified. The members of the open-source version of the "process" class are –

1. Name – Name of the process
2. Process Type – The types of processes are
3. OUTPUT: processes that represent the output of the LCA mdoel.
4. PRIMARY_ENERGY: processes that represent primary energy sources like Coal, Natural gas etc
5. SEC_ENERGY: processes that conversion of primary energy to some form of secondary energy like diesel from oil etc
6. OTHER, NONE: processes that do not fall into any of the above types
7. Attributes 1 through 15: Members to hold attributes of the process

The methods defined in the open-source version of the "process" class are also made generic in order to operate on any arbitrary process.

In order to define the LCA model, the A matrix, A header, B matrix, B header and F matrix are created as separate spreadsheets in a single Microsoft Excel Workbook. Processes can be added to the LCA model by just adding rows and columns to the A header-matrix pair or the B header-matrix pair. When a process needs to be added to A, the attributes are entered as a new row in the A header. The "Name" is the 1st attribute and is mandatory to define the process. All other attributes are optional and are provided to be used by an LCA system-scale model to uniquely identify the process.

Object-oriented Merging is the last step to create a system-scale model. The open-source version of the “merge” program uses the open-source version of the “process” class. The algorithm used is same as what is shown in Figure 34. The method in the “process” class to compare two process objects is made generic in order to compare any attributes.

Results

Twenty-one subsystem-scale LCA models were developed using the data from (Hertwich et al. 2015). Each subsystem-scale LCA model represents an electricity generation technology. The models were merged to create a system-scale model with 537 processes in the **A** matrix representing different energy and material processes and 60 processes in the **B** matrix representing different emissions processes. LCA assessment and ERR computation is performed on the subsystem-scale models and on the system-scale model after merging. The results of the LCA assessment are present in the s vector and the g vector for the energy demand present in the **f** vector. The **s** vector contains the materials, fuels and primary energy feedstock required to meet the energy demand. The **g** vector contains the emissions resulting from emissions resulting from electricity generation to meet the demand.

RESULTS FROM SUBSYSTEM-SCALE LCA AND ERR COMPUTATION

Material usage for a number of materials like aluminum, concrete, iron, copper, etc are computed for each technology using the integrated LCA model. A number of environmental impacts like Green House Gas emissions (GHG), Particulate Matter (PM), Volatile Organic Compounds (VOC), Oxides of Nitrogen (NOx) etc are also computed using the integrated LCA model. Aluminum and GHG are taken as an example in this section because these were included directly and modeled in all the subsystem-scale models (and not from Ecoinvent). The usage of Aluminum for every electricity generation technology is shown in Figure 22. Other materials like iron, cement, copper etc are available for some models but not available for some models because of the use of Ecoinvent data in the data from (Hertwich et al. 2015). CO_2 equivalent greenhouse gas emissions is measured by adding the amount of CO_2 emissions, methane and NO_2. The

GHG emissions are shown in Figure 23. Other emissions like VOC, PM, Carbon monoxide and water vapor are also computed but these are not available for all the subsystem-scale models.

The energy return ratios are computed for every technology using the integrated LCA model. Table 2 shows the Total Energy Output, Total Waste Heat, and Total Waste Heat from Feedstock. The efficiency for the conversion processes for each LCA model is also provided in the Table 2 and is obtained from data provided by supplementary information of (Hertwich et al. 2015).

Table 3 shows the results of the NER and NEER values (Region: US and Year: 2010) computed using (Arvesen and Hertwich 2015) for all electricity generation technologies LCA models developed in this thesis.

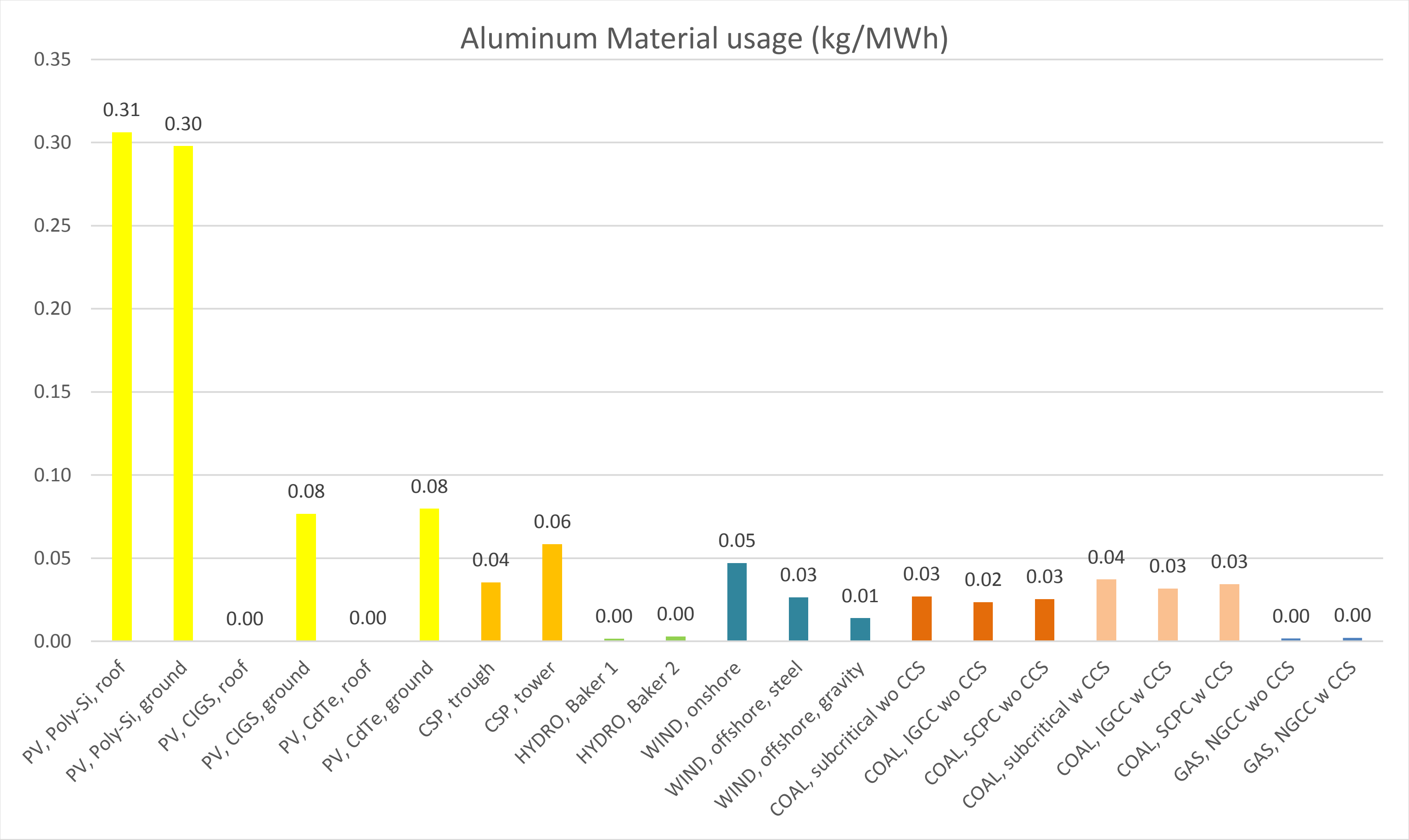


Figure 22: Subsystem-scale Aluminum Material Usage (Region: US, Year: 2010)

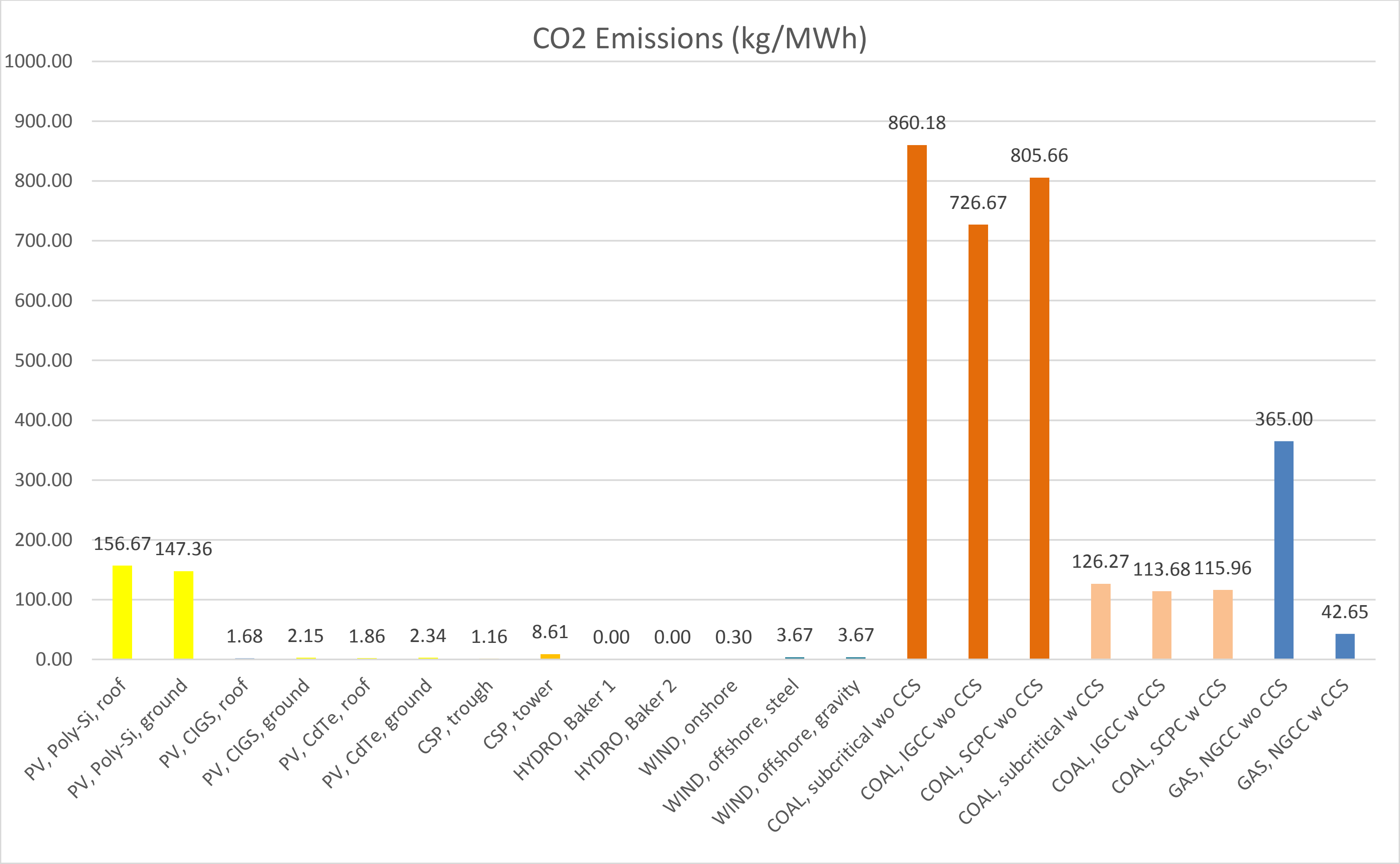


Figure 23: Subsystem-scale GHG Emissions (Region: US, Year: 2010)

	η	Total Energy Output (MJ)	Total Waste Heat (MJ)	Total Waste Heat from Feedstock (MJ)	NER	NEER	GER	GEER
PV, Poly-Si, roof	NA	3.6	1.5088	0.00	2.39	2.39	3.39	3.39
PV, Poly-Si, ground	NA	3.6	1.4106	0.00	2.55	2.55	3.55	3.55
PV, CIGS, roof	NA	3.6	0.0252	0.00	142.86	142.86	143.86	143.86
PV, CIGS, ground	NA	3.6	0.8032	0.00	4.48	4.48	5.48	5.48
PV, CdTe, roof	NA	3.6	0.0453	0.00	79.47	79.47	80.47	80.47
PV, CdTe, ground	NA	3.6	0.8481	0.00	4.24	4.24	5.24	5.24
CSP, trough	NA	4.61E+10	4.42E+09	0.00	10.43	10.43	11.43	11.43
CSP, tower	NA	4.08E+10	5.46E+09	0.00	7.48	7.48	8.48	8.48
HYDRO, Baker 1	NA	8.33E+11	6.67E+09	0.00	124.79	124.79	125.79	125.79
HYDRO, Baker 2	NA	4.54E+11	4.91E+09	0.00	92.45	92.45	93.45	93.45
WIND, onshore	NA	3.6	9.2458	0.00	0.39	0.39	1.39	1.39
WIND, offshore, steel	NA	3.6	4.1409	0.00	0.87	0.87	1.87	1.87

Table 2 continued on next page

WIND, offshore, gravity	NA	3.6	4.1409	0.00	0.87	0.87	1.87	1.87
COAL, subcritical wo CCS	0.382	3.6	6.204	5.8241	0.58	9.48	1.58	10.48
COAL, IGCC wo CCS	0.436	3.6	4.9761	4.6569	0.72	11.28	1.72	12.28
COAL, SCPC wo CCS	0.407	3.6	5.5856	5.2452	0.64	10.58	1.64	11.58
COAL, subcritical w CCS	0.272	3.6	10.1771	9.6353	0.35	6.64	1.35	7.64
COAL, IGCC w CCS	0.322	3.6	7.962	7.5455	0.45	8.64	1.45	9.64
COAL, SCPC w CCS	0.294	3.6	9.1004	8.6449	0.40	7.90	1.40	8.90
GAS, NGCC wo CCS	0.556	3.6	4.4625	2.8748	0.81	2.27	1.81	3.27
GAS, NGCC w CCS	0.474	3.6	5.8378	3.9949	0.62	1.95	1.62	2.95

Table 2: Subsystem-scale Energy Return Ratios Results (using Method 1) (Region: US, Year: 2010)

Technology	CED (MJ/KWh)	Waste heat from Primary Conversion Process (MJ/KWh)	Fuel Input for Primary Conversion Process (MJ/KWh)	Total Methane emitted (kg/KWh)	Energy lost (MJ) (methane heat value 55.5 MJ/kg)	NER	NEER
PV, Poly-Si, roof	0.8656	0	0	1.764E-06	9.79E-05	4.16	4.16
PV, Poly-Si, ground	0.8808	0	0	2.360E-06	1.31E-04	4.09	4.09
PV, CIGS, roof	0.3058	0	0	1.901E-08	1.06E-06	11.77	11.77
PV, CIGS, ground	0.3756	0	0	8.028E-07	4.46E-05	9.58	9.59
PV, CdTe, roof	0.2343	0	0	2.107E-08	1.17E-06	15.36	15.36
PV, CdTe, ground	0.3008	0	0	8.319E-07	4.62E-05	11.96	11.97
CSP, trough	0.3641	0	0	3.450E-08	1.91E-06	9.89	9.89
CSP, tower	0.6399	0	0	9.732E-08	5.40E-06	5.63	5.63

Table 3 continued on next page

HYDRO, Baker 1	1.9264	0	0	1.368E-11	7.59E-10	1.87	1.87
HYDRO, Baker 2	0.1391	0	0	2.508E-11	1.39E-09	25.89	25.89
WIND, onshore	0.1704	0	0	3.422E-09	1.90E-07	21.13	21.13
WIND, offshore, steel	0.2489	0	0	2.137E-08	1.19E-06	14.47	14.47
WIND, offshore, gravity	0.2544	0	0	2.137E-08	1.19E-06	14.15	14.15
COAL, subcritical wo CCS	9.838	6.18	9.96	1.130E-05	6.28E-04	0.37	-29.59
COAL, IGCC wo CCS	8.468	4.938	8.718	1.056E-05	5.87E-04	0.43	-14.37
COAL, SCPC wo CCS	9.226	5.56	9.34	2.976-07	1.65E-05	0.39	-31.57
COAL, subcritical w CCS	14.16	10.15	13.93	1.543E-05	8.57E-04	0.25	15.75
COAL, IGCC w CCS	11.42	6.663	10.443	3.748E-07	2.08E-05	0.32	3.67
COAL, SCPC w CCS	13.05	9.08	12.86	1.158E-06	6.43E-05	0.28	18.82
GAS, NGCC wo CCS	8.03	3.59	7.37	8.575E-09	4.76E-07	0.45	5.45
GAS, NGCC w CCS	9.519	4.819	8.599	9.967E-09	5.53E-07	0.38	3.91

Table 3: NER and NEER using Method 2 (Arvesen and Hertwich 2015) (Region: US, Year: 2010)

RESULTS FROM SYSTEM-SCALE LCA AND ERR COMPUTATION

The system-scale integrated LCA model contains all the processes from 21 subsystem-scale LCA models. The demand for the system-scale LCA model is obtained using electricity generation mix provided by the International Energy Agency (IEA) Blue map scenario for 2050 (IEA 2010) similar to the demand used in (Hertwich et al. 2015). Table 4 shows the demand of electricity from various generation technologies derived from the Blue map scenario for the year 2050 (IEA 2010). The electricity demand from various electricity generation technologies for the year 2050 is added to the F vector of the system-scale LCA model. The LCA assessment and ERR computation is performed using the system-scale LCA model. Table 5 shows selected materials and selected emissions required to meet the supply.

The Efficiency, Waste Energy and Feedstock matrices are merged into the system-scale LCA model. ERR computation is performed on the system-scale LCA model. The Table 6 shows the results of the ERR computation.

Electricity Generation Technology	Electricity Demand (TWh)
PV, Poly-Si, roof	247.9
PV, Poly-Si, ground	247.9
PV, CIGS, roof	1053.5
PV, CIGS, ground	1053.5
PV, CdTe, roof	1053.5
PV, CdTe, ground	1053.5
CSP, trough	123.9
CSP, tower	123.9
HYDRO, Baker 1	2667
HYDRO, Baker 2	2667
WIND, onshore	1638
WIND, offshore, steel	1638
WIND, offshore, gravity	1638
COAL, subcritical wo CCS	1275
COAL, IGCC wo CCS	1275
COAL, SCPC wo CCS	1275
COAL, subcritical w CCS	1529
COAL, IGCC w CCS	1529
COAL, SCPC w CCS	1529
GAS, NGCC wo CCS	4283
GAS, NGCC w CCS	1815

Table 4: System-scale Electricity Demand for 2050 scenario (Year: 2050)

Materials	
Aluminum	24.1 Million Metric tonnes/yr
Copper	1.3 Million Metric tonnes/yr
Emissions	
CO2 Equivalent	85868.6 Million Metric tonnes/yr
Particulate matter (< 2.5 microns)	36.4 Million Metric tonnes/yr

Table 5: System-scale Material usage and emissions (Year: 2050)

Total Energy Output	1.033 x 10^{16} MJ
Total Waste Heat	4.5191 x 10^{15} MJ
Total Waste Heat from Feedstock	4.1618 x 10^{15} MJ
Net Energy Ratio	2.2852
Net External Energy Ratio	28.909
Gross Energy Ratio	3.2852
Gross External Energy Ratio	29.909

Table 6: System-scale Energy Return Ratios (Year: 2050)

Discussion

The data obtained from (Hertwich et al. 2015) uses inputs from the Ecoinvent database. The LCA models developed using the data from (Hertwich et al. 2015) contain processes that represent the inputs from Ecoinvent. However, because of lack of access to the Ecoinvent during the development of this research, all the elements of the column (except the diagonal elements) of the **A**-matrix representing an Ecoinvent process are set to zero. This means, to produce a unit of output from the Ecoinvent process, there are no material or energy inputs required and there are no emissions from these processes. In other words, some energy and other inputs required to produce these materials are not accounted for in the system-scale LCA model. Therefore, the material usage and emissions reported by the subsystem-scale and system-scale LCA models developed in this research are under-counted. However, using the "General primary input" and the "Electricity Supply mix" processes, we have attempted to resolve the problem and attempt to consider all direct and indirect energy sources.

Figure 24 shows a comparison of Aluminum usage between the results obtained by LCA assessment developed in this thesis to the Aluminum usage reported by (Hertwich et al. 2015). The usage of Aluminum (Figure 22) per MWh obtained from the LCA assessment of every electricity generation technology is less than the Aluminum usage per MWh reported in (Hertwich et al. 2015) because of the exclusion of Ecoinvent data from our models. However, the trend of Aluminum usage among the different models appears to be the same as the results from (Hertwich et al. 2015). For example, the usage of Aluminum for electricity generation from Solar PV roof-mounted is less than the usage of Aluminum for electricity generation from IGCC Coal in the results from this thesis and from (Hertwich et al. 2015). Figure 25 shows a comparison of CO_2 equivalent GHG emissions between the results obtained by LCA assessment of the system-scale LCA model developed in this thesis to the CO_2 equivalent GHG emissions reported by (Hertwich et al. 2015). The CO_2 equivalent GHG emissions per MWh of electricity (Figure 23) computed from the subsystem-scale LCA assessment for most of the electricity generation technology is less than the CO_2 equivalent GHG emissions per MWh of electricity reported in (Hertwich et al. 2015) because of exclusion of Ecoinvent data from our models. However, the trend of CO2 equivalent GHG emissions among the different models appears to be the same as the results in (Hertwich et al. 2015). The GHG for Solar PV Poly-Si calculated from our model is greater than (Hertwich et al. 2015) because the Solar PV Poly-Si uses electricity from the grid. Because of the use of the "Electricity Supply from Grid", this electricity will inturn be supplied by the combination of mainly Natural gas (35%) and Coal (40%) sources. As a result, the GHG for Solar PV Poly-Si in our model is high. In (Hertwich et al. 2015), it not clear what is the supply mix of grid electricity used.

Most of the subsystem-scale LCA models developed in this thesis are based on outputting a unit of electricity. However, the subsystem-scale CSP and Hydro LCA models are based on outputting a CSP or Hydro power plant respectively. For CSP, two types of power plants are modelled and a lifetime of 30 years is assumed similar to the (Hertwich et al. 2015). Supplementary data of (Hertwich et al. 2015) also provides annual electricity generation from these plants. Using the lifetime and the annual electricity generation, the material use and emissions per unit of electricity is computed for CSP subsystem-scale LCA models. For Hydro, two reservoirs are modelled and a lifetime of 80 years is assumed similar to the (Hertwich et al. 2015). Supplementary data of (Hertwich et al. 2015) also provides the capacity of the power plants. The capacity factor of about 0.5 is assumed for the power plants. Using the capacity, capacity factor and the lifetime of the power plant, material use and emissions per unit of electricity is computed for Hydro subsystem-scale LCA models.

Table 7 shows a comparison of the energy return ratios computed using (Arvesen and Hertwich 2015) method (Method 2) with the energy return ratios computed using the methodology developed in this thesis (Method 1 based on (Brandt et al. 2013)). NER, for all fossil fuel technologies and some renewable technologies (CIGS-ground, CdTE-ground, Hydro and CSP), from Method 1 and Method 2 match closely but the NER computed from Method 1 is greater than NER computed from Method 2. This is possibly due to the exclusion of energy sources like diesel, oil or natural gas in some models because they are input in physical units (like kg, m^3) instead of purely energy units (like MJ). Including these energy sources into the Waste heat vector will decrease the NER computed by Method 1. The inclusion of the energy sources that are provided in physical units is taken as a goal of future research. NER computed using Method 1 for some technologies (PV Poly-Si, CIGS-ground, CdTE-ground, Wind) is lower than the NER computed using Method 2. One possible reason for this is the use of electricity from the grid and the difference in the supply mix assumptions between the Method 1 and 2.

The NEER from Method 2 has resulted in values that are not in the expected range of acceptable values. NEER for Subcritical wo CCS, IGCC wo CCS and SCPC wo CCS are negative numbers (-29.59, -14.37 and -31.57 respectively), which is not expected. The NEER is –ve because the denominator of Equation (17) is –ve. The factors of that make up the denominator are the CED, Fuel input and the Energy Lost and they are used directly from the data provided by supplementary information of (Hertwich et al. 2015). The main reason the CED is –ve is because CED is greater than the calculated Fuel input. CED cannot be greater than the Fuel input to maintain energy balance. Therefore, there is reason to believe that there are inconsistencies in the CED and Fuel input factors that arise possibly from the large inconsistencies of the heating values of Coal from Ecoinvent. (Arvesen, personal email communication, Nov 09 2015).

The results from the system-scale LCA assessment is mainly driven by the energy mix in the demand matrix of the system-scale LCA model. The system-scale LCA results are not compared with (Hertwich et al. 2015) because the energy mix used for system-scale LCA computation is not known. For example, the Blue map 2050 scenario demand of electricity from Wind is 4916 TWh (IEA 2010). However, it does not provide the demand from onshore wind, offshore wind – steel foundation and offshore wind – gravity foundation. In this thesis, the demand for electricity from different sources of wind-based electricity generation is split evenly (33% each). However, the demand for electricity from different sources of wind-based electricity generation used in (Hertwich et al. 2015) is unknown. Another example is, even though the total amount of energy from coal is known, the energy demand for IGCC wo CCS, Supercritical wo CCS, Supercritical w CCS and Subcritical wo CCS is not known. Even though the energy mix is made as similar to (Hertwich et al. 2015) as possible, difference in energy mix within the same type of electricity producing technology may result in a large difference in material use and environmental impact. For example, differences in demand from PV Poly-Si will have big differences in the Aluminum usage because of the relatively high Aluminum per MWh for PV Poly-Si. Also, the difference in assumptions like the capacity factor and the electricity gird’s supply mix will have impact on the material use and environmental impact results. Additionally, when the material use and environmental results from the same integrated LCA model aligns with (Hertwich et al. 2015), it can be assumed that, when the supply mix is the same, the results from our system-scale LCA analysis should also align with (Hertwich et al. 2015). Therefore, the system-scale material use and environmental impact results are not compared to (Hertwich et al. 2015).

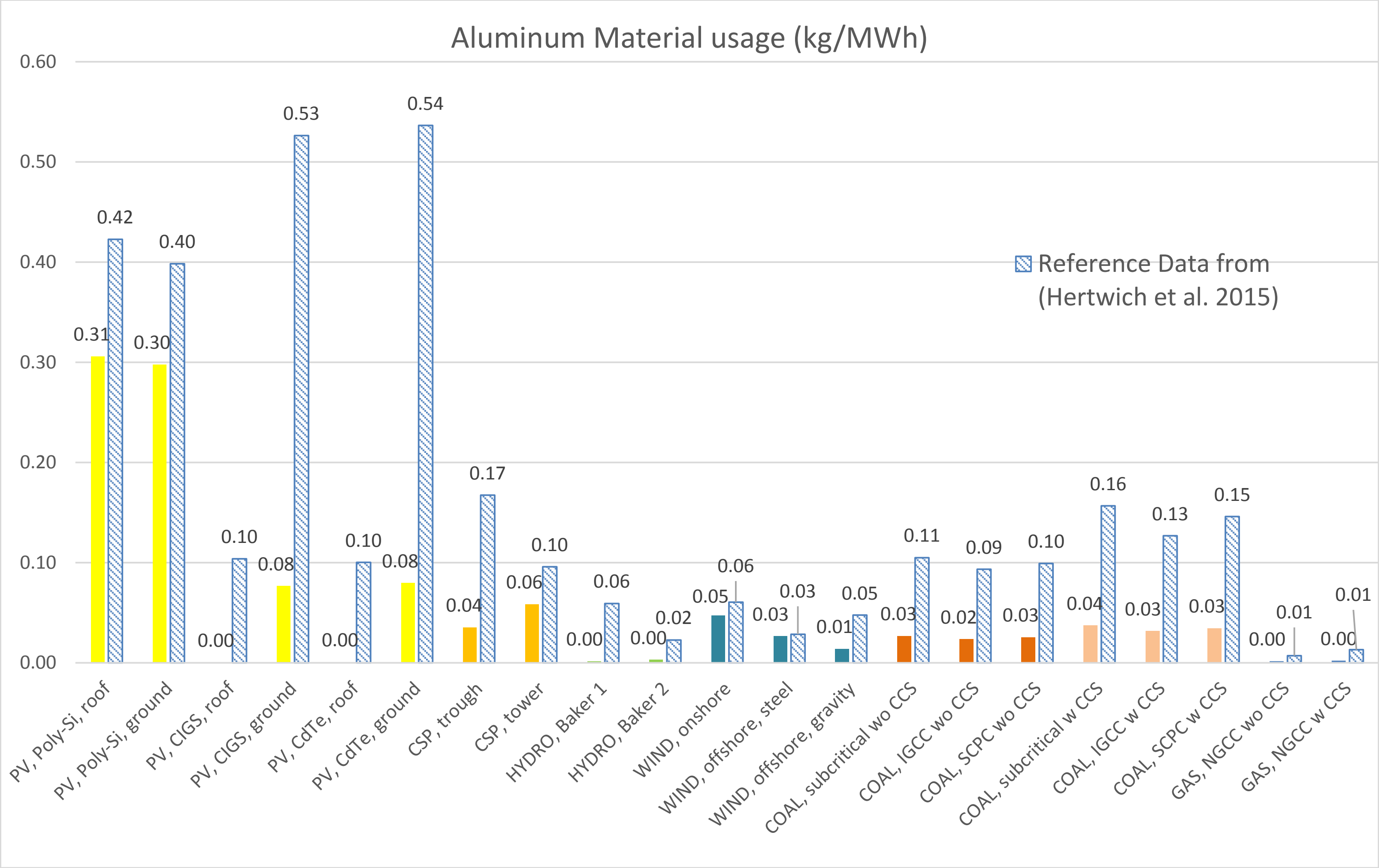


Figure 24: Comparison of Aluminum usage with (Hertwich et al. 2015) (Region: US, Year: 2010)

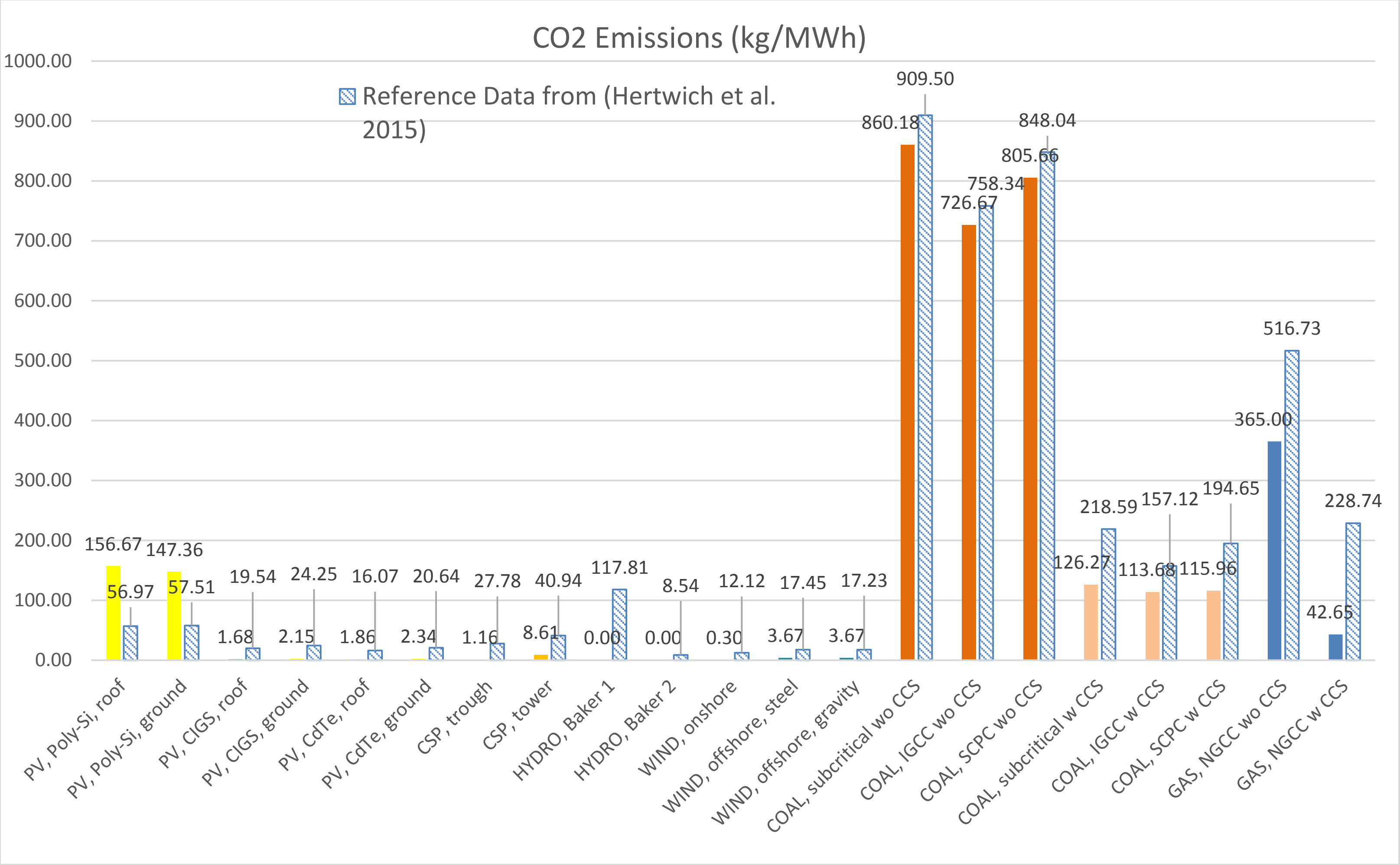


Figure 25: Comparison of GHG emissions with (Hertwich et al. 2015)(Region: US, Year: 2010)

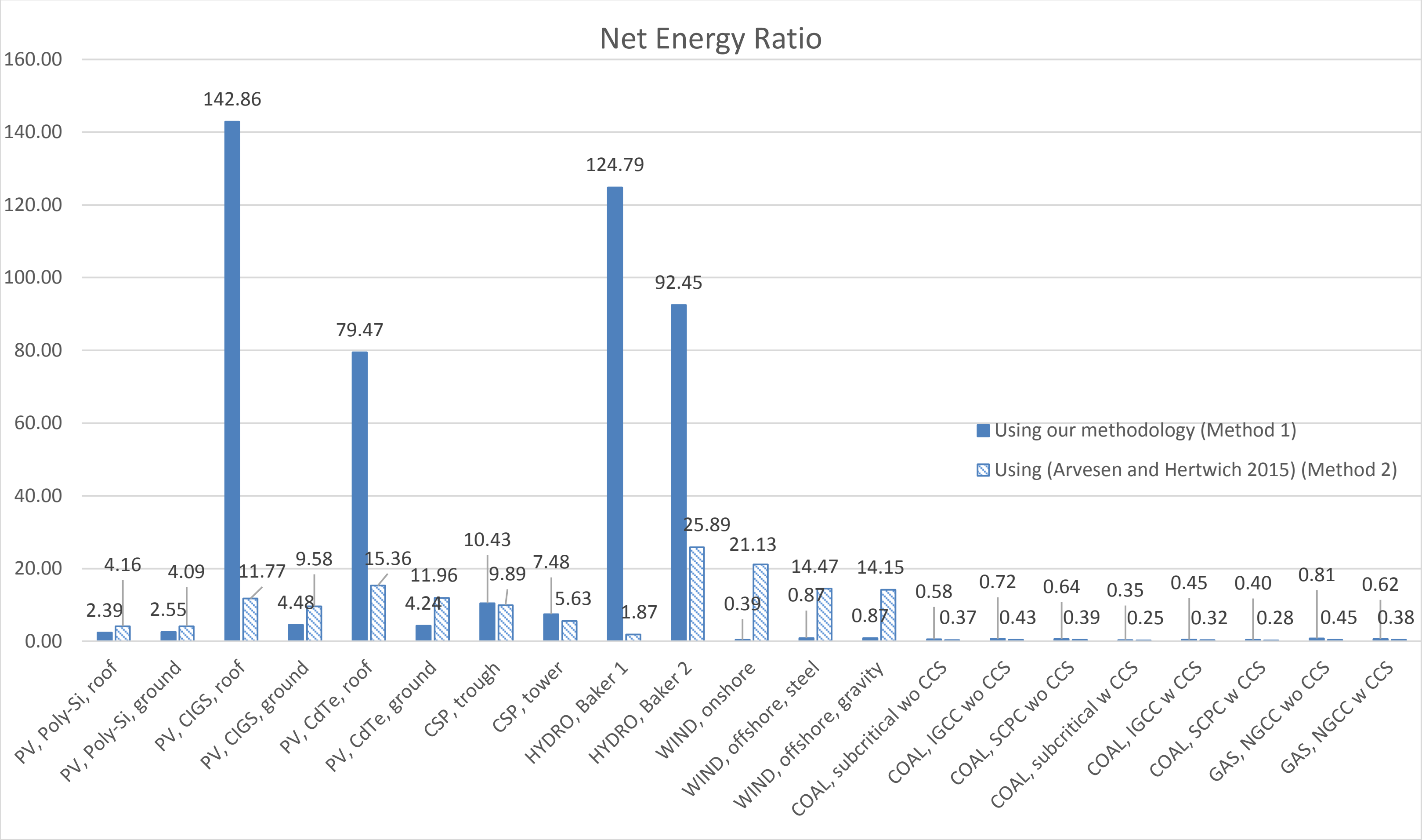


Figure 26: NER Comparison

	Our method (Method 1)		ERR from CED (Method 2)	
	NER	NEER	NER	NEER
PV, Poly-Si, roof	2.39	2.39	4.16	4.16
PV, Poly-Si, ground	2.55	2.55	4.09	4.09
PV, CIGS, roof	142.86	142.86	11.77	11.77
PV, CIGS, ground	4.48	4.48	9.58	9.59
PV, CdTe, roof	79.47	79.47	15.36	15.36
PV, CdTe, ground	4.24	4.24	11.96	11.97
CSP, trough	10.43	10.43	9.89	9.89
CSP, tower	7.48	7.48	5.63	5.63
HYDRO, Baker 1	124.79	124.79	1.87	1.87
HYDRO, Baker 2	92.45	92.45	25.89	25.89
WIND, onshore	0.39	0.39	21.13	21.13
WIND, offshore, steel	0.87	0.87	14.47	14.47
WIND, offshore, gravity	0.87	0.87	14.15	14.15
COAL, subcritical wo CCS	0.58	9.48	0.37	-29.59
COAL, IGCC wo CCS	0.72	11.28	0.43	-14.37
COAL, SCPC wo CCS	0.64	10.58	0.39	-31.57
COAL, subcritical w CCS	0.35	6.64	0.25	15.75
COAL, IGCC w CCS	0.45	8.64	0.32	3.67
COAL, SCPC w CCS	0.40	7.90	0.28	18.82
GAS, NGCC wo CCS	0.81	2.27	0.45	5.45
GAS, NGCC w CCS	0.62	1.95	0.38	3.91

Table 7: Comparison of ERR results from Method 1 and Method 2

Conclusion

The methodology presented in this thesis has resulted in the development of a system-scale LCA model that includes 21 different electricity producing technologies. The programs developed using this methodology have enabled LCA assessment and energy return ratio computations at system-scale and subsystem-scale. Two methodologies were developed to calculate energy return ratios using the LCA models. An open source methodology was developed to enable improvement of the system-scale LCA model.

The absence of data from Ecoinvent database has resulted in undercounting the material use and energy factors viz. waste heat, total energy consumed and total energy from feedstock. The energy ratios calculated using the bottom-up methodology developed in this thesis (Method 1) are not as complete as they can be because of absence of inputs from the Ecoinvent database. This results in many energy inputs missing and therefore, the energy ratios are not actually representative of the real system. The energy ratios calculated by Method 1 are higher than the energy ratios of the real system. The goal of future research is to complete the model by adding data that is not currently included.

The computation of energy ratios using CED values (Method 2) was performed because the energy factors are undercounted in Method 1, due to the exclusion of inputs from the Ecoinvent database. However, some NEER values calculated using Method 2 have resulted in negative values. Negative values for energy ratios are incorrect and represents energy imbalance, which is physically not possible. The factors that make up the denominator of the NEER (Equation 17) is a negative number. The factors that make up the denominator are the CED, Fuel input and the Energy Lost, and they are used directly from the data provided by (Hertwich et al. 2015). The main reason the CED is negative is because CED is greater than the calculated Fuel input. CED cannot be greater than the Fuel input to maintain energy balance. This indicates there are inconsistencies in the relationships between CED and waste heat values provided by (Hertwich et al. 2015). Reconciling the energy balance information for full LCAs that use Ecoinvent and economic input information, is thus a priority for future research.

Appendix A

BACKGROUND OF OBJECT ORIENTED METHODOLOGY

Objected Oriented Methodology (OOM) is a programming model where the functionality is implemented using objects as the fundamental data structures to store data and logical procedures. OOM provides significant benefits compared to conventional sequential programming models. Apart from some advantages related to actual process of developing the source code and managing the source code, OOM provides important advantages like reusability, interoperability and scalability. Objects are defined by defining classes. Classes can be reused either by adding more members and methods to the class or by using inheritance. Inherited objects from same parent class provide interoperability. Large data sets and complex functions can be implemented using OOM and modern simulators run object oriented programs very efficiently due to the use of garbage collection. Therefore, programs developed using OOM are scalable.

The fundamental data structure of an OOM program is an object. An object is defined by a class. An instance of a class is an object. Objects contain members and methods. Members are variables that are used to hold data. Methods are functions that are used to implement arithmetic and logical operations on the data of the object. Objects can hold objects of the same kind or different kind using handles. This is an important property that enables programmers to build scalable models.

The system under consideration is designed as a system of inter-dependent processes. Each process is a finite system that consumes some inputs and produces some output. In order to represent a system, a number of processes are defined with well-defined relationships in terms of the inputs and outputs of between processes.

LCA PROCESS AS AN OBJECT

A process is the fundamental data-structure using which the LCA model is developed. In the context of a class-based object oriented methodology, the process is defined by a class and the class includes all the attributes of a LCA process. Some of the basics attributes of the process object are shown in Table 8. A process can have additional attributes as shown in Table 9. Using all the attributes of a process, the process can be uniquely identified in a LCA model.

Basic Process Attributes	**Description**
Name	Name of the process
Output Unit	Unit of the output generated by the process
Output Quantity	For a given object, the amount of the output for which the process is characterized

Table 8: Basic Process Attributes

Other Process Attributes	**Description**
Process Type	Output/Input/Natural resources etc
Category	Process Category (Construction, materials etc)
Subcategory	Process Sub-category (concrete generation, metal extraction etc)
Source of Data	Own model/Ecoinvent etc

Table 9: Other Process Attributes

LCA SYSTEM AS TREE OF PROCESSES

A LCA system is modelled as a collection of a number of process objects. There is a finite relationship between processes in terms of the inputs and outputs of the processes. A given process of a system can have inputs from a number of processes. In order to represent this relationship in the object oriented methodology, the process is designed to have one or more children process objects. These children processes are linked to the parent using object handles. An object handle is used to represent the relationship between the child process object from a parent process object. It is used to programmatically link the parent object and the child object. Table 10 shows the additional attributes that are required to store data related to child processes. Table 11 shows an example of a system with multiple processes and their relationships.

Process Attributes for representing Children	**Description**
Handles for Children	Handles for Child process objects
Number of Children	Number of Child processes

Table 10: Process Attributes for Representing Children

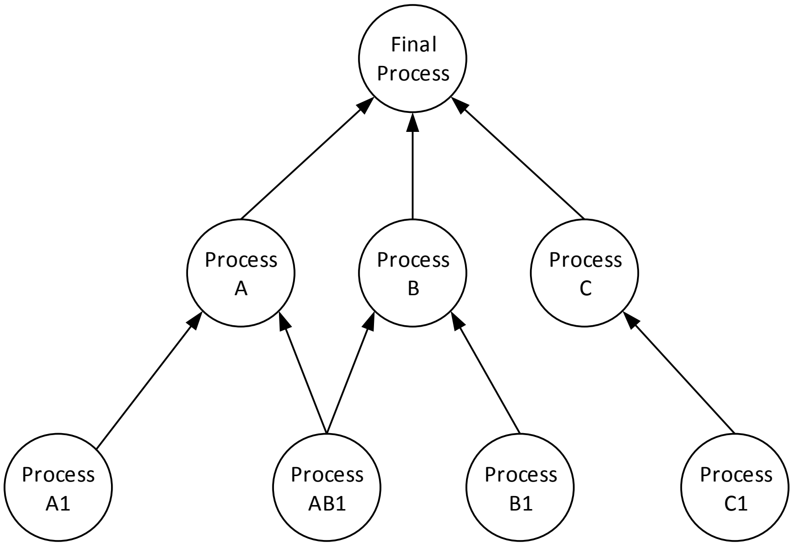


Figure 27: LCA Process Tree

When modeling a LCA system, a final process-object is created first and it represents the process which produces the final unit of output under analysis. This final process-object will have one or more children, each one providing some amount of the input to be used in the final process-object. These process-objects are represented as Process A, B and C in the Figure 27. These children process-objects will in-turn have their own children process-objects that represents inputs going into the child process. These process-objects are represented as Process A1, AB1, B1 and C1. Therefore, the LCA system is built as a tree of process-objects with the top node of the process-object representing the final process of the system.

Figure 28 shows an example LCA system modeling generation of electricity from coal. The LCA system has 7 processes. The LCA model of the system depicting the various relationships between processes is shown in Table 11. The descriptions of the processes are –

1. Final process: Final process represents the unit of electricity generated by the coal generation process. It has three children viz. Plant Infrastructure, Plant Operation and Cabling. These child processes represent the inputs to the Final process to generate a unit of electricity which is primary outputs of the model.

2. Plant operation process: The Plant operation represents the process that involves conversion of coal to electricity. Plant operation process has one child viz. the Coal Extraction process.

3. Plant Infrastructure: Plant infrastructure represents the requirement of having to construct the coal plant. In this example, it has one child process viz. the aluminum required to developing the plant infrastructure.

4. Cabling: Cabling represents the process of installing cables in order to provide electricity produced by the plant to the grid. It has one child process viz. the aluminum required to developing cabling.

5. Aluminum Generation: This process represents the generation of aluminum. This process has one child process viz. the electricity input required for aluminum generation.

6. Coal Extraction: This process represents the extraction of coal to be used in the Plant operation. This process has one child process viz. the coal from the coal-mine.

7. Coal from Mine: This process represents the coal extracted from the mine. This process does not have any children and it represents one of the primary energy inputs to the LCA system.

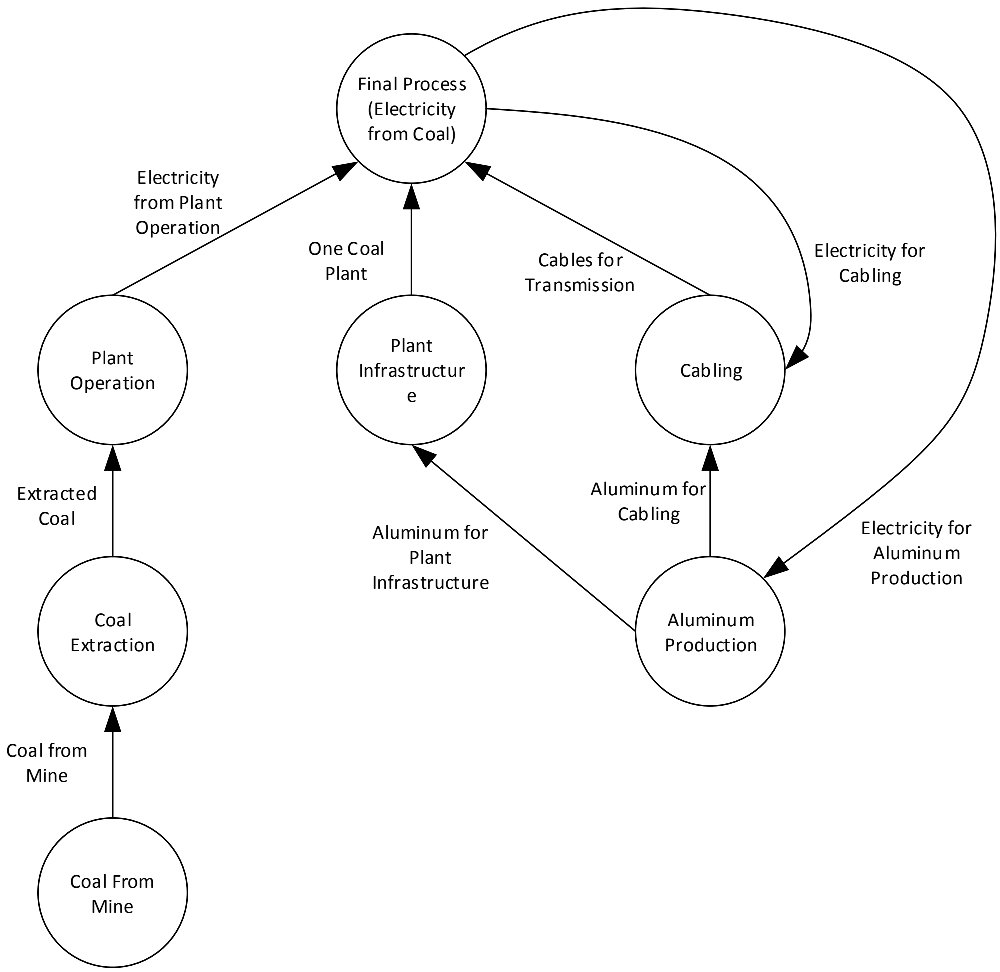


Figure 28: Cyclic LCA System Tree for Electricity Generation from Coal

Name	**Output**	**Output Unit**	**Output Quantity**	**Number of children**	**Children**
Final Process - Electricity from Coal	Electricity	KWh	1	3	Plant Infrastructure, Plant Operation, Cabling, Cabling
Plant Operation	Electricity	KWh	1	1	Coal Extraction
Plant Infrastructure	Coal Plant	coal plant	1	1	Aluminum Extraction
Cabling	Aluminum	Kg	1	1	Aluminum Extraction
Aluminum Generation	Aluminum	Kg	1	1	Electricity from Coal
Coal Extraction	Coal	Kg	1	1	Coal from Mine
Coal from Mine	Coal	Kg	1	0	NA

Table 11: Processes of LCA System for Electricity Generation from Coal

LCA models will have relationships from outputs of the some processes to inputs to some processes. In a LCA model tree, if there is a relationship between a parent process and its child process such that, the output of a given parent process is an input to a child process then, the model is said to be cyclic tree. The computational complexity when creating and parsing models will be very high because of the cyclic nature of the LCA models.

In order to reduce the computational complexity, the model is converted to a flattened model. The computation complexity is reduced because, in the flattened model, there is only one level of relationship for a given process. Processes have children but do not have grandchildren. The flattened model will have a set of handles to all the processes modeled in the system. The cyclic LCA model shown in example Figure 28 is converted to a flattened model shown in Figure 29.

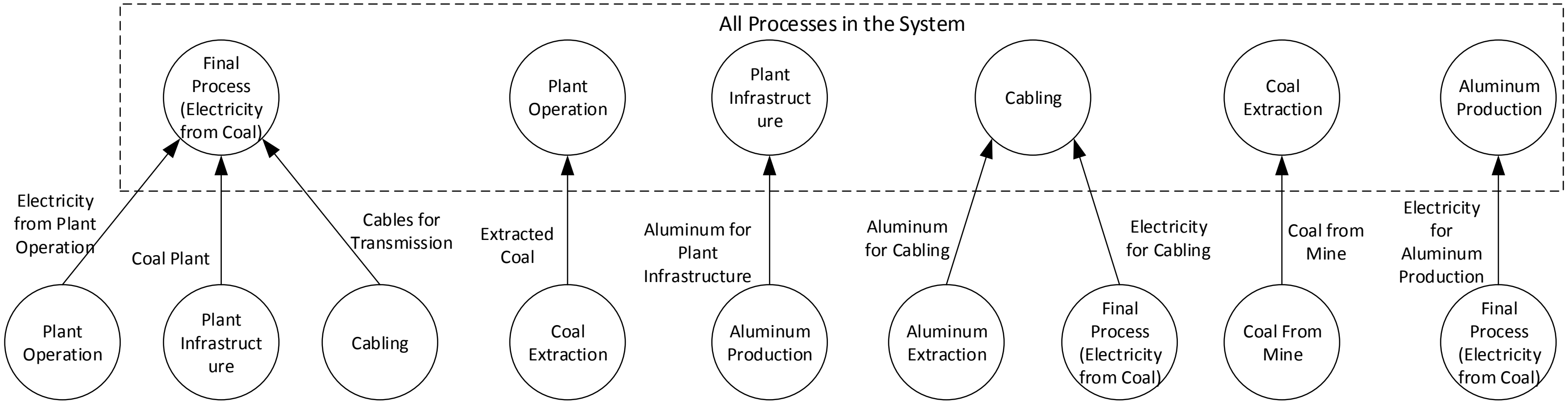


Figure 29: Flattened LCA System for Electricity Generation from Coal

BUILDING THE LCA SYSTEM-SCALE MODEL

The system-scale model is designed as a set of individual LCA subsystem-scale models using a bottom-up methodology. Each subsystem-scale represents a different electricity generation technology. The subsystem-scale models are first built and these subsystem-scale models are then merged in order to obtain a single, unified system-scale model. Data from (Hertwich et al. 2015) is used for building subsystem-scale models.

Creating subsystem-scale LCA models

A subsystem-scale LCA model has a restricted scope. It is modeled as a set of processes pertaining to the output under consideration at the subsystem-level boundary. An algorithm shown in Figure 30 is used to create the subsystem-scale model. All the processes of the subsystem are converted to process-objects starting from the final process of a subsystem. Each process-object, after creation, is added to a list of processes. The list of processes contains all processes that belongs to the subsystem.

The algorithm to convert a process to a process-object is shown in Figure 31. For a given process of a subsystem, the process-object is first created using object oriented methodology by creating an instance of the process class. After the object is created, all the required attributes of the process are set using the process's attributes. For all the inputs to the process, child processes are created. The child processes are created by creating instances of the process class. The process contains a list of handles of the child processes and a variable to denote the number of children. The quantity of the input required to generate one unit of the output is copied into the child process along with other attributes of the child process. The handle of this child process is added to the list of children in the parent process. The number of children for the process is also incremented. Because the subsystem LCA model is flattened, there is no requirement to create the grandchildren of the process under consideration.

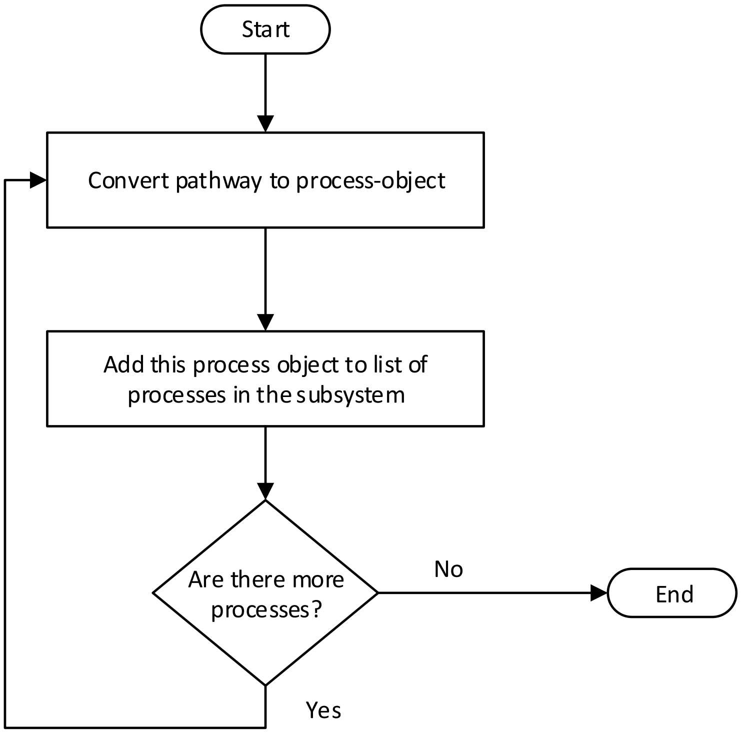


Figure 30: Algorithm to create process-objects in a LCA model

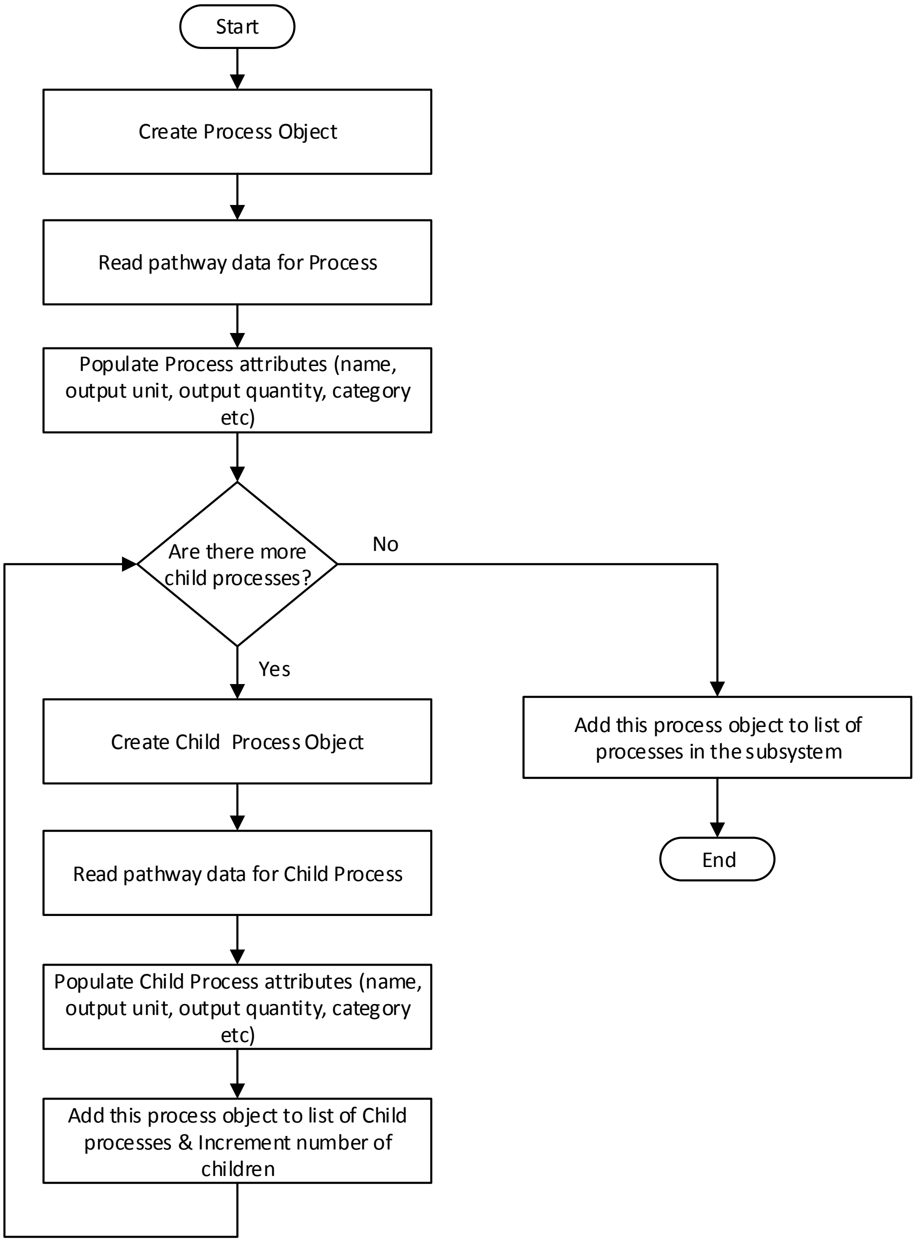


Figure 31: Algorithm to Convert a Process to a Process-Object

Conversion of subsystem-scale LCA tree to matrices

The processes of the subsystem-scale LCA model is converted to the A and B header-matrix pairs format using an algorithm that processes one process at a time. The A and B matrices are used to LCA assessment and ERR computation (Heijungs and Suh 2002). The A matrix is the technology matrix and it contains economic flows that include energy and material flows. The B matrix is the intervention matrix and it contains environmental flows that include emissions flows (Heijungs and Suh 2002).

Creating the A header-matrix pair

The A header-matrix pair contains all the energy and material processes a given subsystem. The A header-matrix pair has two parts – A-header and the A-matrix. The A-header is a list of process-objects whose data is present in the matrix – one for every row in the A-matrix. Because the A-matrix is a square matrix, the A-header is also the header every column in the A-matrix. The A-matrix is the actual matrix that contains the quantities. The separation of the header and matrix facilitates easier implementation using tools like Matlab. The rows represent processes that provides inputs to the processes present in the columns.

The algorithm to update the A header-matrix pair is shown in Figure 32. Before the algorithm starts, the A-matrix is an empty matrix and the A-header is an empty list of processes. The final process is first added to the A-header. The final process will be the first row and first column of the A matrix. All the children of the final process are then added as rows to the A header-matrix pair. It is important to note that all the quantities from the child processes are added in the column of the parent process. Following the final process, all the other processes of the LCA subsystem and their children are added or updated into the A header-matrix pair.

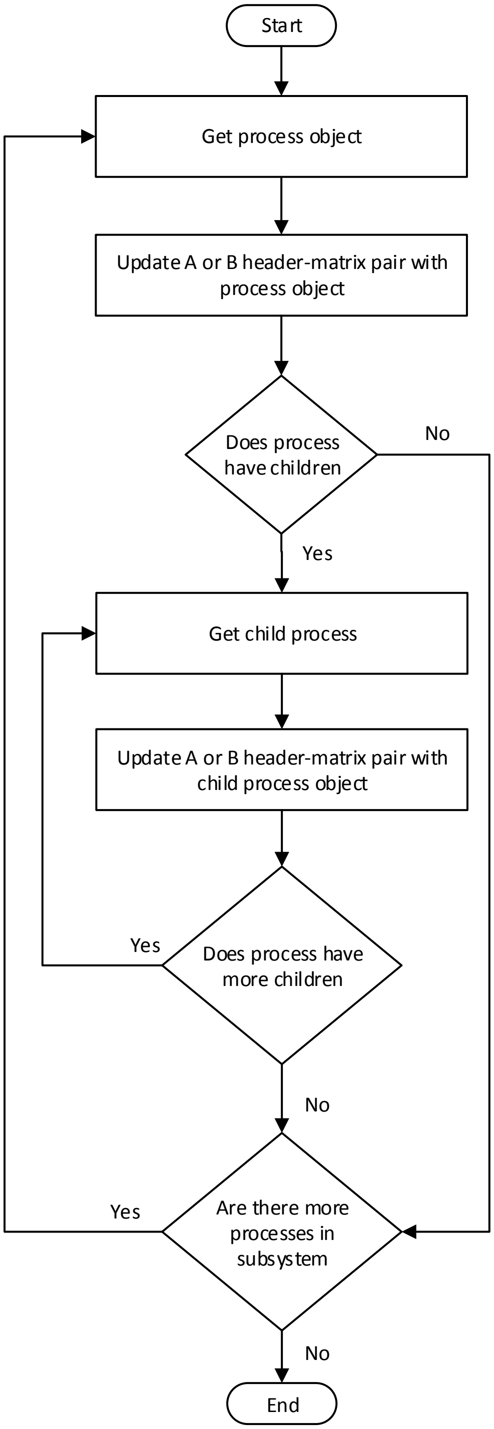


Figure 32: Algorithm to Convert all process-objects to A & B header-matrix pair

The algorithm to update or add a given process to the A header-matrix pair is shown in Figure 33. When a parent process is being updated or added into the A header-matrix pair, a column is added to the A-matrix and all elements of the column are set to 0. The addition of the column is not performed for child processes. The quantities from child processes are added into the same column as the parent. A variable called col_num is maintained to keep track of which column the data is updated into. Processes that deal with material and energy outputs are added into the A header-matrix pair. Emissions processes and waste heat processes are updated into the B header-matrix pair. Process attributes like process-type can help distinguish the type of the process and is used to decide if the process is to updated into the A header-matrix pair or the B header-matrix pair.

If the destination of the process is the A header-matrix pair, then the A-header is searched to see if the process being added is already present as a row. If the row is not present, a new row, with all zeros, is added to the A matrix and the process is also added to the A header list. If the row is already present, the index of the row is recorded in a variable called row_num. For cases where the row is not present, the row_num will be set equal to the index of the latest row that was added to the A header-matrix pair.

Lastly, the A matrix is updated using the indices row_num and col_num. The element of at A(row_num, col_num) is set equal to the output quantity of the process being added. If the process is providing an input to another process, then the output quantity being added is negative.

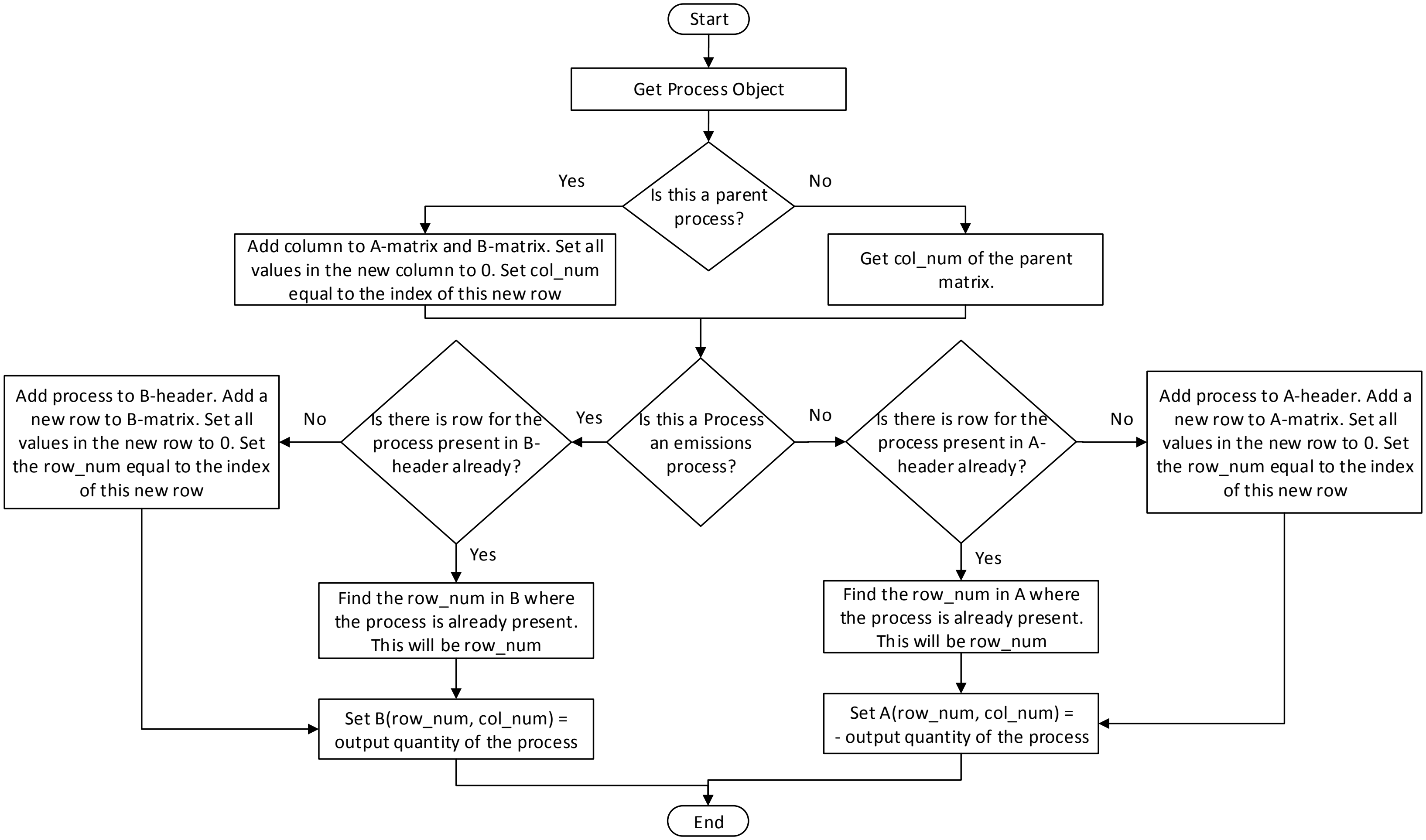


Figure 33: Algorithm to Update the A & B header-matrix pair for a process

Creating the B header-matrix pair

Creating the B header-matrix is very similar to how the A header-matrix pair is created. All processes with outputs representing emissions or waste heat is added to the B header-matrix pair. The algorithm to update or add a given process to the B header-matrix pair is shown in Figure 33. This algorithm is the same as the one used when adding processes to the A header-matrix pair. The key difference is, the addition of columns to the B header-matrix pair depends on the addition of A header-matrix pair. For a given parent process, the columns are added to B header-matrix pair when columns are added to the A header-matrix pair.

Lastly, when the B matrix is updated using the indices row_num and col_num, the element of at B(row_num, col_num) is set equal to the output quantity of the process being added. Because the process is an emissions or a waste heat process, the quantity is positive.

Creating the F vector

F vector represents the demand of output from each process. The F vector will be created by the system modeler and will be an input to the model. The entries of the F vector will represent the rows of the A matrix. Therefore, the A header is used to represent the processes of the F vector. A separate header is not required.

Object based merging to create system-scale models

Large systems will have numerous processes. A large system-scale LCA model will include numerous relationships that will hard to model at the system level. In order to solve this problem, the large system-scale model is designed using a bottom-up approach. The models are designed and developed at the sub-system level. Because of the restricted scope at the subsystem-scale, all the inter-process relationships are added into the subsystem-scale model. The individual subsystem-scale models are then merged to obtain a large system-scale model on which LCA can be performed.

In the bottom-up approach is shown in Figure 35, multiple subsystem-scale models might share some common processes. For example, a subsystem LCA model for Electricity from Coal and Electricity from Wind share a process that represents generation of steel. When merging the subsystem models, processes that are common between the models are identified. For the processes that are common, the values in the A and B matrices are appropriately set when merging. For identifying common processes, brute force comparison can be performed yielding very high runtimes for big models. Instead, merging is done by saving the indices of processes in the models that are being merged and selectively extracting models processes that are not common.

The merge is run on two subsystem-scale LCA models viz. input1 and input2 to produce a merged output. The algorithm to merge two subsystem-scale LCA models is shown in Figure 34. Additional handles called “in1_idx” and “in2_idx” are created in each process object. “in1_idx” represents the index of each process in the input1 process list. “in2_idx” represents the index of each process in the input2 process list. “output_idx” represents the index of each process in the output process list. The A header-matrix pairs of the input models are read by the algorithm. Lists of process objects are created while reading the A header-matrix and B header-matrix pairs for each input. The in1_idx while reading the input1 A header-matrix pair. The in2_idx is updated while reading the input2 A header-matrix pair. Common processes between input1 and input2 are identified. All processes from input1 and input2 are added to the output process list. Common processes are only added from input1. Finally, the output A matrix is created using the in1_idx and in2_idx of each processes in the output process list. Merging of B matrices is also done using the same algorithm.

A process attribute called “demand” is added to the process object. In order to merge the F matrices, the demand value for every process in A-header is read into the corresponding “demand” attribute of process object. After merging the matrices and when output header-matrix pair is being created, a new F matrix is created using the “demand” attributes of all processes in the output process list.

Merge is designed to take two input subsystem-scale LCA models at a time. A merge tree is created in order to merge a large number of models. In a merge tree, the output of merge from one level is used as an input to the next level. Merge trees help to keep the complexity manageable because larger matrices are created and handled while merging towards the top of the tree.

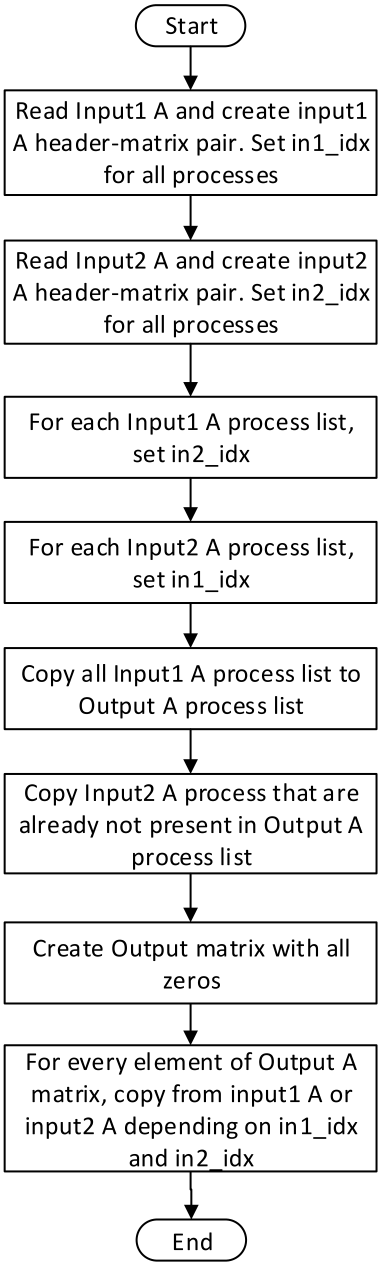


Figure 34: Algorithm to merge two subsystem-scale LCA models

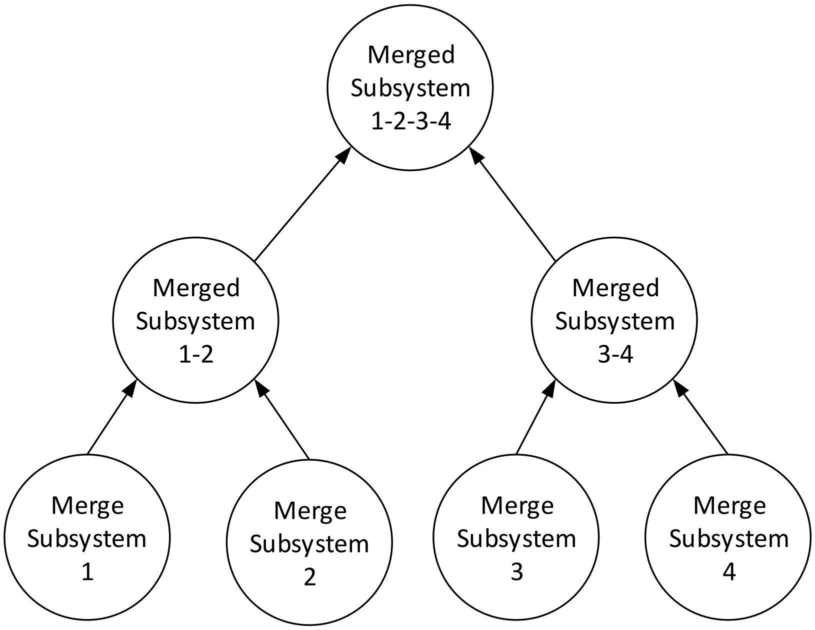


Figure 35: Merge tree

PROCESS DEFINITION

A class called “process” is defined and it becomes the fundamental data structure used to create process objects that represent all processes for all electricity generation technologies. Having objects of the same class for all processes enables easy interoperability between code that handles multiple susbsystems (like merging and net-energy analysis code). The “process” class has two important constituents – members and methods. The members represent the attributes of a given process that the object is presenting. In order to fully capture all the data from the (Hertwich et al. 2015) source technology files, the following attributes are defined in the class definition (similar to attributes present in the processes from (Hertwich et al. 2015)) –

1. Source
2. Name

3. LCA category
4. LCA Sub-category
5. LCA Activity
6. Complete name
7. Internal process code
8. Product code
9. IO Classification/CPA code
10. Temporal lifetime
11. First year of Expense
12. Discount factor
13. Regional representativeness
14. Country Code
15. Quantity
16. Quantity Unit
17. Quantity Min
18. Quantity Max
19. Unit Factor
20. Standard Unit

Other members of the class include

1. proc_handle: this is a list of handles to all the children of this process
2. proc_index: It is an integer that represents the number of children
3. filename, sheetname, process name: Strings that represent some basic technology file information.
4. in1_idx and in2_idx : these are handles used for merging operations.
5. parse_state and next_parse_state: These are used for the parsing state machine.

Methods are functions that are implemented in the class. Some common functionality is implemented as methods in the class. Some of the important methods of the "process" class are –

1. parse: This is the main function that reads the sheet and creates a process object for every process. It also reads the processes that are inputs to a given process and creates the child process objects and list of children. This function is used extensively when reading data from the spreadsheets.
2. compare: It compares two process objects and provides a result to denote if the process objects represent the same process. The function compares all the relevant attributes to determine if the processes are the same. This function is used extensively when creating matrices and during merging operations.
3. Copy_process_values: this function is called by the parse() function. It is used to copy a line from the excel sheet to the attributes.

Other methods that help in making the overall code more organized, more readable and more manageable are added in the "process" class definition.

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